List of Publications (R.Ahuja)

Publications : Total 1070 publications in international journals.

(6 in Nature, 1 in Science, 25 in PNAS, 35 in PRL, 4 in Nano-Letters, 4 in Ang.Chem., 3 in Adva. Funct. Mat., 1 in Energy & Envior. Sci. & 14 in Nano Energy, 1 in Materials Today, 1 in Science Advances, 20 in J. of Mater. Chem. A, 3 in Chem. Mat., 1 in ACS Energy Letters). More than 26 Cover pages of journals.
Total No. of Citations (Google Scholar) : more than 40000, H-index (Google Scholar) : 92, i-10 index (Google Scholar) : 679

1.R. Ahuja, A.K. Solanki, T. Nautiyal, and S. Auluck
Fermi surface of the noble metals
Journal of Physics Pramana **32**, 831 (1989).

2.R. Ahuja, A.K. Solanki, and S. Auluck
Effect of pressure on the Fermi surface of noble metals
Phys. Rev. B **39**, 9806 (1989).

3.R. Ahuja, A.K. Solanki, and S. Auluck
Fermi surface characteristics of Palladium
*Physica status solidi (b)***160**, 549 (1990).

4.A.K. Solanki, R. Ahuja, and S. Auluck
Fermi surface and mass enhancement factor for Niobium
Physica status solidi (b) **162**, 497 (1990).

5.R. Ahuja, A.K. Solanki, and S. Auluck
Effect of hydrostatic pressure on the Fermi surface of Pd and Pt
*Phys. Rev. B***43**, 2401 (1991).

6.R. Ahuja, A.K. Solanki, and S. Auluck
Fermi surface properties of Platinum
Physica status solidi (b) **168**, 509 (1991).

7.A.K. Solanki, R. Ahuja, and S. Auluck
Fermi surface characteristics and mass enhancement factor for Tantalum
Journal of Physics Pramana **38**, 189 (1992).

8. R. Ahuja, A.K. Solanki, and S. Auluck
Fermi surface of ferromagnetic nickel

Physica Scripta **45**, 621 (1992).

9.A.K. Solanki, R. Ahuja, and S. Auluck
Fermi surface properties of Vanadium
Physica B **179**, 257 (1992).

10.R. Ahuja, A.K. Solanki, and S. Auluck
Effect of pressure on the Fermi surface of ferromagnetic Nickel
*Phys. Rev. B***46**, 3785 (1992).

11.R. Ahuja, A.K. Solanki, and S. Auluck
Effect of strain on the Fermi surface of the noble metals
*Phys. Rev. B***48**, 1373 (1993).

12.A.K. Solanki, R. Ahuja, and S. Auluck
Influence of hydrostatic pressure on the Fermi surface of Nb,V, and Ta
*Physica Status Solidi (b)***182**, 377 (1994).

13.R. Ahuja, A.K. Solanki, T. Nautiyal, and S. Auluck
Effect of pressure on the Fermi surface of transition metals
Recent Trends in High Pressure Research (Oxford and IBH
Publishing Co., 1992), p.86.

14.R. Ahuja, A.K. Solanki, and S. Auluck
Fermi surface of copper under strain
*Recent Trends in High Pressure Research (*Oxford and IBH
Publishing Co., 1992), p.91.

15.A.K. Solanki, R. Ahuja, and S. Auluck
The Fermi surface of VB transition metals ; under hydrostatic pressure
Recent Trends in High Pressure Research(Oxford and IBH
Publishing Co., 1992), p.94.

16.Rajeev Ahuja, John.M. Wills, Börje Johansson and Olle Eriksson
Crystal structures of Ti, Zr, and Hf under compression ; theory
*Phys. Rev. B***48**, 16269 (1993).

17.O. Eriksson, J. M. Wills, P. Söderlind, J. Melsen, R. Ahuja,
A. M. Boring and B. Johansson
Crystallographic Phase Transitions in Actinide Metals as a Function of Pressure
J. Alloys and Compounds **213/214**, 268 (1994).

18.P. Söderlind, R. Ahuja, O. Eriksson, B. Johansson, and J. M. Wills
Theoretical predictions of structural phase transitions in Cr, Mo, W
*Phys. Rev. B***49**, 9365 (1994).

19.R. Ahuja, P. Söderlind, J. M. Wills, B. Johansson, and O. Eriksson
Platinum at Ultrahigh Pressure
High Pressure Research **12**, 161 (1994).

20.R.Ahuja, S.Auluck, B. Johansson, and M.S.S. Brooks
Electronic Structure, Magnetism and Fermi Surfaces of Gd and Tb
*Phys. Rev. B***50**, 5147 (1994).

21.R.Ahuja, S.Auluck, B. Johansson, and M.A.Khan
Optical Properties of PdO and PtO
*Phys. Rev. B***50**, 2128 (1994).

22.R. Ahuja, P. Söderlind, J.Trygg, J.Melsen, J. M. Wills, B. Johansson
and O. Eriksson
Influence of pseudo core valence-band hybridization on the crystal-structure phase
stabilities of transition metals under extreme compressions
*Phys. Rev. B***50**(*Rapid Communication*), 14690 (1994).

23.P. Söderlind, R. Ahuja, O. Eriksson, J. M. Wills and B. Johansson
Crystal Structure and Elastic Constant Anomalies in the Magnetic
3*d* Transition Metals
*Phys. Rev. B***50**, 5918 (1994).

24.R.Ahuja, S.Auluck, P.Söderlind, O.Eriksson, J.M.Wills and B. Johansson
The Fermi surface of noble metals : full potential, generalized gradient approximation
*Phys. Rev. B***50**, 11183 (1994).

25.R.Ahuja, S.Auluck and Börje Johansson
Effect of pressure on the Fermi surface of Ni ; Non-local potential
Physica Scripta **50**, 573 (1994).

26.R.Ahuja, S.Auluck, O.Eriksson, J.M.Wills and B. Johansson
Fermi surface of alkali metals using the full potential linear muffin
tin orbital method and the generalized gradient approximation
*Phys. Rev. B***50**, 18003 (1994).

27. R.Ahuja, S.Auluck, Börje Johansson and M.A.Khan
Anisotropic Dielectric Response of Ferromagnetic Cobalt
J. Magn. Mag. Materials(JMMM) **140-144**, 89 (1995).

28.R.Ahuja, S.Auluck, J.Trygg, O.Eriksson, J.M.Wills and B.Johansson,
Electronic Structure of Graphite : Effect of hydrostatic pressure
Phys. Rev. B **51**, 4813 (1995).

29.Börje Johansson, Rajeev Ahuja, Olle Eriksson and J. M. Wills
The anomalous fcc crystal structure of Thorium metal
Phys. Rev. Lett. **75**, 280 (1995).

30.O.Eriksson, R.Ahuja, A.Ormeci, J.Trygg, O.Hjortstam, P.Söderlind, B.Johansson and J.M.Wills
Bulk and surface magnetism and interplaner spacings in Gd from first principles calculations
Phys. Rev. B. **52**, 4420 (1995).

31. R.Ahuja, P.A.Bruhwiler, J.M.Wills, B.Johansson, N.Mårtensson, and O.Eriksson,
Theoretical and Experimental Study of the Graphite 1*s* X-ray Absorption Edges
Phys. Rev. B**54**, 14396 (1996) .

32.P.A.Bruhwiler, P.Kuiper, O.Eriksson, R.Ahuja and S.Svensson
Core Hole Effects in Resonant Inelastic X-ray Scattering (RIXS) of Graphite
Phys. Rev. Lett. **76**, 1761 (1996).

33. Rajeev Ahuja, Olle Eriksson, J.M.Wills and Börje Johansson
Theoretical Confirmation of the High Pressure Simple Cubic Phase in Calcium
Phys. Rev. Lett. **75**, 3473 (1995).

34. Rajeev Ahuja, Olle Eriksson, J.M.Wills and Börje Johansson
Structural and Elastic Properties of Cubic TiC, TiN and TiO
P*hys. Rev. B***53**, 3072 (1996).

35. M.Pajda, R.Ahuja, O.Eriksson, J.M.Wills, H.Figiel, A.Paja and B.Johansson
Calculations of the magnetic properties of YMn_2 and its hydrides
J. Phys. C. **8**, 3373 (1996).

36. R.Ahuja, O.Eriksson, J.M.Wills, A.B.Belonoshko, L.S.Dubrovinsky and B.Johansson
A New High Pressure Phase of Silica
Accepted for publication in *Nature*.

37. R.Ahuja, P.James, O.Eriksson, J.M.Wills and B.Johansson
A theoretical study of the pressure-induced structural phase transition in CdTe
*Physica Status Solidi (b)***199**, 75 (1997).

38. A.Delin, O.Eriksson, R.Ahuja, T.Gasche, M.S.S.Brooks and B.Johansson
Optical properties of the Group IVB refractory-Metal Compounds
*Phys. Rev. B***54**, 1673 (1996).

39.R.Ahuja, S.Auluck, J.M.Wills, M.Alouani, B.Johansson and O.Eriksson
Optical Properties of Graphite from First Principles Calculations
*Phys. Rev. B***55**, 4999 (1997).

40.R.Ahuja, S.Auluck, O.Eriksson, J.M.Wills and B.Johansson
Electronic and Optical Properties of HgI_2
*Phys. Rev. B***54**, 10419 (1996).

41.A.B.Belonoshko and R.Ahuja

Embedded-atom molecular and lattice dynamics study of Iron
Phys. Earth Planet. Inter. **102**, 171 (1997).

42. L.S.Dubrovinsky, S.K.Saxena, P.Lazor, R.Ahuja, O.Eriksson, J.M.Wills and B.Johansson,
Experimental and theoretical identification of a new high-pressure phase of silica,
Nature **388**, 362 (1997).

43.P.Ravindran, A.Delin, R.Ahuja, B.Johansson, S.Auluck, J.M.Wills and O.Eriksson
Optical Properties of monoclinic SnI_2 from relativistic first principles theory
*Phys. Rev. B***56**, 6851 (1997).

44.J.Johansson, O.Eriksson, B.Johansson, L.Fast and R.Ahuja
First principles study of Mn up to extreme pressures
*Phys. Rev. B***57**, 10989 (1998).

45.L.Fast, R. Ahuja, L.Nordström, J.M. Wills, B. Johansson and O. Eriksson
Anomaly in c/a ratio of Zn under pressure
Phys. Rev. Lett. **79**, 2301 (1997).

46.L.S.Dubrovinsky S.K.Saxena, R.Ahuja and B.Johansson
Theoretical study of $MgSiO_3$ at conditions of Earth's Lower Mantle
*Geophys. Res. Lett.***25**, 4253 (1998).

47.R.Ahuja, S.Auluck, O.Eriksson, J.M.Wills and B.Johansson
Electronic and Optical Properties of InP
Solid State Comm. **104**, 249 (1997).

48.R.Ahuja
Theoretical High Pressure Phase study of Alkali Hydrides
Advances in High Pressure Science and Technology,
(Universities Press Limited, 1997), p.281.

49.R.Ahuja, A.B.Belonoshko and B.Johansson
Melting and Liquid structure of Aluminum oxide using Molecular Dynamic Simulation
*Phys. Rev. E***57**, 1673 (1998).

50.Rajeev Ahuja, Börje Johansson, John. M. Wills, and Olle Eriksson
On the semi conducting state and structural properties of YH_3 from First principles theory
Appl. Phys. Lett. **71**, 3498 (1997).

51.R.Ahuja, S.Auluck, O.Eriksson and B.Johansson
Calculated Electronic and Optical Properties of Graphite Intercalation Compound :LiC_6
J. Phys. C:Condens.Matt. **9**, 9845 (1997).

52.Rajeev Ahuja, S. Auluck, Olle Eriksson, John. M. Wills, and Börje Johansson
Electronic and Optical Properties of Solar Energy Material : $CuGaS_2$
Solar Energy Materials and Solar Cells **53**, 357 (1998).

53.P.Ravindran, L. Nordström, R.Ahuja, J.M.Wills, B.Johansson and O.Eriksson
Theoretical investigation of high pressure phases of Ce
*Phys. Rev. B***57**, 2091 (1998).

54.Rajeev Ahuja, Olle Eriksson, J.M.Wills and Börje Johansson
Theoretical High Pressure Phase study of Cesium Hydride
J. Phys. C : Letter to Editor **10**, L153 (1998).

55.R.Ahuja, B.Johansson,J.M.Wills and O.Eriksson
Structural Phase Transformations in alkaline earth oxide and chalcogenides at high pressure : Theory
Advances in High Pressure Research in Condensed Matter,
(NISCOM, New Delhi, 1997), p.250.

56.R.Ahuja, L.Fast, J.M. Wills, B. Johansson and O. Eriksson
Elastic and High Pressure properties of ZnO
J. Appl. Phys. **83**, 8065 (1998).

57.R. Ahuja, O. Eriksson, J.M. Wills and B. Johansson
High pressure phase study of Sr
*Phys. Rev. B***58**, 8152 (1998).

58.R.Ahuja, O. Eriksson and B. Johansson
Theoretical Search for the CrB-type High Pressure Phase in LiH, NaH, KH and RbH
Physica B **265**, 87 (1999).

59.Rajeev Ahuja, Olle Eriksson and Börje Johansson
Electronic and Optical properties of FeS_2 and CoS_2
*Philosphical Mag. B***78**, 475 (1998).

60.B. Holm, Rajeev Ahuja, Y.Yourdshahyan, B.Johansson and B.I.Lundqvist
Electronic and Optical properties of α- and κ-Al_2O_3
*Phys. Rev. B***59**, 12777 (1999).

61.H.Hua, Y.K.Vohra, J.Akella, S.T.Weir, Rajeev Ahuja and B.Johansson
Theoretical and Experimental studies on Gadolinium at Ultra High Pressure
Rev. High Pressure Sci. Technol.**7**, 233 (1998).

62.P.Ravindran, A.Delin, P.James, B.Johansson, J.M.Wills, Rajeev Ahuja and O.Eriksson
Magnetic, optical and magneto-optical properties of MnX (X=As, Sb and Bi) from full potential calculations
*Phys. Rev. B***59**, 15680 (1999).

63.B.Hjörvarsson, J.H.Guo, G.Andersson, R.C.C.Ward, R. Ahuja, O. Eriksson, C.Sathe, A.Agui, S.M.Butorin and J.Nordgren
Measurements and calculations of the electron density in yttrium and its hydrides
J. Phys. C : Letter to Editor **11**, L119 (1999).

64.G.Guemmaz, A.Mosser, Rajeev Ahuja and B. Johansson
Elastic properties of sub-stoichiometric TiC. Comparison of FP-LMTO calculations and experimental results
*Solid State Commun.***110**, 299 (1999).

65. N.A.Dubrovinska, L.S.Dubrovinsky,S.K.Saxena, R.Ahuja and B.Johansson
High Pressure studies of TiC
J. Alloys and Comp. **289**, 24 (1999).

66.U.Haussermann, S.I.Simak, Rajeev Ahuja, B.Johansson and S.Lidin
The Origin of the distorted closed-packed elemental structure of In
Angew. Chem. Intl. Engl. **38**, 2017 (1999).

67.U.Haussermann, S.I.Simak, Rajeev Ahuja and B.Johansson
A unified Bonding Picture for the Metallic Triel Elements
Angew. Chem. Intl. Engl. **39**, 1246 (2000).

68.R. Ahuja, O. Eriksson and B. Johansson
Theoretical High Pressure studies of Silicon-VI
P*hys. Rev. B***60**, 14475 (1999).

69.B.Holm and R. Ahuja
Ab initio calculation of elastic constants of SiO_2 stishovite and α-quartz
J. Chem. Phys. **111**, 2071 (1999).

70.P.James, O.Eriksson, R.Ahuja and I.A.Abrikosov
Structural stability and mixing energy of 3d alloys: a comparision of theoretical methods
Proceedings of the Moscow International Symposium on Magnetism (MISM'99) pp. 109 (1999).

71.A.B.Belonoshko, R.Ahuja, O.Eriksson and B.Johansson
Quasi *ab initio* Molecular Dynamic Study of Cu melting
*Phys. Rev. B***61**, 3838 (2000).

72.A.B.Belonoshko, R.Ahuja and B.Johansson
Mechansim for the κ-Al_2O_3 and α-Al_2O_3 and the stability of κ-Al_2O_3 under volume expansion
Phys. Rev. B **61**, 3131 (2000).

73.A.B.Belonoshko, R.Ahuja and B.Johansson
Molecular dynamics of LiF melting
Phys. Rev. B **61**, 11928 (2000).

74.G.Gutierrez, A.B.Belonoshko, R.Ahuja and B.Johansson
Structural properties of liquid Al_2O_3: A molecular dynamics study
*Phys. Rev. E***61**, 2723 (2000).

75a.R. Ahuja, O. Eriksson, J.M. Wills and B. Johansson
Electronic Structure of Ti_3SiC_2
Appl. Phys. Lett. **76**, 2226 (2000).

75b.One of the figure (Fig.5) of above paper has been appeared on the cover page of the book entitled ``*2002 Graduate Programs in Physics, Astronomy, and related Fields*'' compiled by the **American Institute of Physics**.

76.A.B.Belonoshko, R.Ahuja and B.Johansson
Quasi *ab initio* molecular dynamic study of hcp iron melting
Phys. Rev. Lett. **84**, 3638 (2000).

77.P.Söderlind, R. Ahuja, O. Eriksson, B. Johansson and J.M. Wills
Delocalization and predicition of a new phase in americium :theory
*Phys. Rev. B***61**, 8119 (2000).

78.Y. Meresse, S.Heathman, T.Le Bihan, J.Rebizant, M.S.S.Brooks and R. Ahuja
X-Ray Diffraction Studies of $AuCu_3$ neptunium compounds under pressure
J. Alloys and Comp. **296**, 27 (2000).

79.P. Monachesi, M. Palummo, R. Del Sole, R. Ahuja and O. Eriksson
Optical Properties of Cu-(110) surface
MRS, **579**, 59 (2000).

80.S.I.Simak, U.Haussermann, Rajeev Ahuja, S.Lidin and B.Johansson
Gallium and Indium under High Pressure
Phys. Rev. Lett. **85**, 142 (2000).

81. P.Mohn, P.Weinberger, L.Ujfalussy, O.Eriksson, G.Gutieres, R.Ahuja, and B.Johansson
Mystery of the Alkali metals: Giant moments on Fe and Co on and in Cs films
Phys. Rev. Lett. **85**, 1583 (2000).

82.S.Rekhi, L.S.Dubrovinsky, R.Ahuja, S.K.Saxena and B.Johansson
High Pressure studies of Cr_2O_3
J. Alloys and Comp. **302**, 16 (2000).

83.Rajeev Ahuja
High Pressure Studies of Alkali Metals and Alkali Halides
Sci. Technol. of High Pressure **2**, 639 (2000).

84.Rajeev Ahuja
HIGH PRESSURE STUDIES OF SODIUM AND SILVER HALIDES
High Pressure Research **18**, 131 (2000).

85.S.I.Simak, U.Haussermann, Rajeev Ahuja, S.Lidin and B.Johansson
Gallium under High Pressure
Sci. Technol. of High Pressure **1**, 448 (2000).

86.B.Holm, R.Ahuja, A.B.Belonoshko and B.Johansson
Theoretical investigation of the high pressure phases of carbon dioxide
Phys. Rev. Lett. **85**, 1258 (2000).

87.A.Srivastava, R.K.Singh, R.Ahuja and B.Johansson
Semi magnetic Semiconductor under High Pressure : Phase Transitions from B1-B2 observed under TBP approach
Sci. Technol. of High Pressure **2**, 830 (2000).

88.B.Holm, R.Ahuja and B.Johansson
Ab initio calculations of the mechanical properties of Ti_3SiC_2
Appl. Phys. Lett. **79**, 1450 (2001).

89.R.Ahuja, O.Eriksson and B.Johansson
Electronic and Optical Properties of $BaTiO_3$ and $SrTiO_3$
J. Appl. Phys. **90** 1854, (2001).

90.L.S.Dubrovinsky, N.A.Dubrovinskaia, V.Swamy, J.Muscat, N.M. Harrison, R.Ahuja, B.Holm and B.Johansson
The Hardest Known Oxide
Nature **410**, 653 (2001).

91.P. Monachesi, M. Palummo, R. Del Sole, R. Ahuja and O. Eriksson
Ab initio-calculated RAS spectra of Cu- and Ag- (110) surfaces
*Phys. Rev. B***64**, 5421 (2001).

92.N.A.Dubrovinskaia, M.Vennstrom, I.A.Abrikosov, R.Ahuja, P.Ravindran, Y.Andersson, O.Eriksson and L.S.Dubrovinsky
Absence of a pressure induced structural phase transition in Ti_3Al up to 25GPa
*Phys. Rev. B***63**, 024106 (2001).

93.Rajeev Ahuja, O.Eriksson and B.Johansson
Theoretical high pressure studies of Cs metal
*Phys. Rev. B***63**, 014102 (2001).

94.Rajeev Ahuja, O.Eriksson and B.Johansson
High Pressure Structural Phase Transition in NaBr and NaI
*Phys. Rev. B***63**, 102105 (2001).

95.A.C. Jenkins, W.M. Temmerman, R. Ahuja, O. Eriksson, B. Johansson and J.M.Wills
The relationship between Interlayer Spacing and Magnetic Ordering in Gadolinium
J. Phys. C **12**, 10441 (2000).

96.Rajeev Ahuja and B.Johansson
Theoretical Prediction of Cmca Phase in Ge under high Pressure

J. Appl. Phys. **89**, 2547 (2001).

97.G.E.Grechnev, H.W.Hugosson, R.Ahuja and O.Eriksson
Structural evolution and hardness of transition metal dioxides at high pressure
High Pressure Phys. Techno. **10**, 38 (2000).

98.N.V. Skorodumova, R. Ahuja, S.I. Simak, I.A. Abrikosov, B. Johansson
and B.I. Lundqvist
Electronic, bonding and optical properties of CeO_2 and Ce_2O_3
from the first principles
*Phys. Rev. B***64**, 5108 (2001).

99.A.B.Belonoshko, R.Ahuja and B.Johansson
High Pressure and temperature melting in metals
High Pressure Phys. Techno. **10**, 100 (2000).

100.R.Ahuja, S.Rekhi S.K.Saxena and B.Johansson
High Pressure structural phase transition in RuO_2 and its geophysical Implications
J. Phys. Chem. Solids **62**, 2035 (2001).

101.S.Rekhi, S.K.Saxena, R.Ahuja and B.Johansson
Experimental and theoretical investigations on the compressibility of
nanocrystalline nickel
J. Material Science **36**, 4719 (2001).

102.R.Ahuja, S.Rekhi and B.Johansson
Theoretical Prediction of Phase Transition in Gold
*Phys. Rev. B***63**, 212101 (2001).

103. C.Persson, A. Ferreria da Silva, R.Ahuja and B.Johansson
Effective electronic masses in wurtzite and zinc-blende GaN and AlN
J. Crystal Growth **231**, 397 (2001).

104.R.Ahuja, B.Holm, A.B.Belonoshko and B.Johansson
Quartz like phases in CO_2 at very high pressure from *ab initio* simulations in *`Frontiers of High Pressure Research II: Application of High Pressure toLow-Dimensional Novel Electronic Materials'*, edited by H.D.Hochheimer, B. Kuchta, P.K.Dorhout and J.L. Yarger, NATO Science Series, (Kluwer Academic Publishers) Vol. **48**, 189 (2001).

105.P. Monachesi, M. Palummo, R. Del Sole, R. Ahuja and O. Eriksson
Optical properties of Cu- and Ag- (110) surfaces from *ab initio* theory in *`Electrons and Photons in Solids'*, edited by G.Grosso, G.L. Rocca and M.Tosi (Scuola Normale Superiore, Pubblicazioni Della Classe Di Scienze Pisa, Italy) page 347 (2001).

106.M.Guemmaz, A.Mosser, R. Ahuja and J.C.Parlebas
Theoretical and experimental investigations on elastic properties of substoichiometric titanium nitrides : Influnce of lattice vacancies
Int. J. Inorg. Materials **3**, 1319 (2001).

107.C.Persson, R.Ahuja, A. Ferreria da Silva and B.Johansson
First-principle calculations of optical properties of wurtzite AlN and GaN
J. Crystal Growth **231**, 407 (2001).

108.A.B.Belonoshko, R.Ahuja and B.Johansson
Molecular Dynamics Study of Melting and fcc-bcc Transitions in Xe
Phys. Rev. Lett. **87**, 165505 (2001).

109.J. R. L. Fernandez, C. Moyses Araujo, A. Ferreira da Silva, J. L. Leite,
Bo E. Sernelius, A. Tabata, E. Abramof, V. A. Chitta, C. Persson, R. Ahuja,
I. Pepe, D. J. As, T. Frey, D. Schikora, and K. Lischka
Electrical resistivity and band-gap shift of Si-doped GaN and Metal-nonmetal transition
in cubic GaN, InN, and AlN systems,
J. Cryst. Growth **231**, 420 (2001).

110. A.B.Belonoshko, G.Guterez, R.Ahuja and B.Johansson
Molecular dynamic simulations of the structure of Y_2O_3 phases using pairwise
interactions
*Phys.Rev. B***64**, 184103 (2001).

111.R.Ahuja and L.S.Dubrovinsky
High pressure structural phase transitions in TiO_2 and synthesis of the hardest known
oxide
J. Phys. C **14**, 10995 (2002).

112.B.Holm, R. Ahuja and B.Johansson
Ab initio calculations of mechanical properties of Ti_3SiC_2
Appl. Phys. Lett. **79**, 1450 (2001).

113. N.A.Dubrovinskaia, L.S.Dubrovinsky, R.Ahuja, J. M. Osorio-Guillen and B.Johansson
Experimental and theoretical Identification of New High Pressure TiO_2 Polymorph
Phys. Rev. Lett. **87**, 275501 (2001).

114.C. Persson, Bo E. Sernelius, A. Ferreira da Silva, R. Ahuja and B.Johansson
Effective electron and hole masses in intrinsic and heavily n-type doped GaN and AlN
J. Phys. C **13**, 8915 (2001).

115.C. Persson, R. Ahuja, A. Ferreira da Silva and B. Johansson
First-principle calculations of dielectric function in cubic and hexagonal InN
J. Phys. C **13**, 8945 (2001).

116.A. Ferreira da Silva, C. Moyses Araujo, C. Persson, Bo E. Sernelius, R.Ahuja and
B. Johansson
Influence of Si doping on optical properties of wurtzite GaN
J. Phys. C **13**, 8891 (2001).

117.C. Persson, R. Ahuja, and B. Johansson

Full band calculation of doping-induced band-gap narrowing in p-type GaAs
Phys. Rev. B **13**, 033201 (2001).

118.K. Dewhurst, R.Ahuja, Sa Li and B.Johansson
Phonons in pressurized Solid Xenon
Advances in High Pressure Science and Technology,
Eds. A.K.Bandyopadhyay, D.Varandani and K. Lal, 184 (2001).

119.A. El. Goresy, M.Chen, P.Gillet, L.Dubrovinsky, G.Graup and R.Ahuja
A natural shock-induced dense polymorph of rutile with alpha-PbO2
in the suevite from Ries crater in Germany
Earth and Planetay Sci. Lett. **192**, 485 (2001).

120. R.Ahuja
A search for new super hard materials using high pressure
Advances in High Pressure Science and Technology,
Eds. A.K.Bandyopadhyay, D.Varandani and K. Lal, 219 (2001).

121.A.B.Belonoshko, O. Le Bacq, R.Ahuja and B.Johansson
Molecular dynamics study of phase transitions in Xe
J. Chem. Phys. **117**, 7233 (2002).

122.R.Ahuja and L.S.Dubrovinsky
High pressure structural phase transitions in TiO_2 and synthesis of the hardest known oxide
J. Phys. C **14**, 10995 (2002).

123.H.W.Hugosson, G.E.Grechnev, R.Ahuja,U.Helmersson, Sa Li and O.Eriksson
Stabilisation of potential superhard RuO_2 phase : A theoretical study
*Phys.Rev. B***66**, 174111 (2002).

124.C.Moyses, J.R.L.Fernandez, A. Ferreria da Silva, I.Pepe, J.R.Leite,
Bo E. Sernelius, A.Tabata, C.Persson, R.Ahuja, D.J.As, D.Schikora and K.Lischka
Electrical Resistivity, MMM transition and Band-gap narrowing of cubic GaN:Si
Microelectronic J. **33**, 365 (2002).

125.R.Ahuja and L.S.Dubrovinsky
Cotunnite-structured titanium dioxide and the hardest known oxide
High Press. Res. **22**, 429 (2002).

126.B.Holm, R. Ahuja, Sa Li and B.Johansson
Theory of the ternary layered system Ti-Al-N
J. Appl. Phys. **91**, 9874 (2002).

127.C. Persson, Bo E. Sernelius, A. Ferreira da Silva, C. Moyses Araujo, R. Ahuja, and B. Johansson
Optical and reduced band gap in n- and p-type GaN and AlN

J. Appl. Phys. **92**, 3207 (2002).

128.J.K. Dewhurst, R.Ahuja, S. Li and B.Johansson
Lattice Dynamics of Solid Xenon Under Pressure
Phys. Rev. Lett. **88**, 075504 (2002).

129.Y. Wang, R.Ahuja and B.Johansson
Melting of Iron and Other Metals at Earth's Core Conditions: A Simplified Computational Approach
Phys. Rev. B **65**, 014104 (2002).

130.Y. Wang, R.Ahuja and B.Johansson
Calculated Hugoniot curves of Porous Metals: Cu, Ni and Mo
in Shock Compression of Condensed Matter-2001 edited by M.D.Furnish, N.N.Thandhani and Y.Horie (American Institute of Physics, 2002), **62,** p.67.

131.J. Schmadt, P.A.Bruwiler, I.Patthey, J.N.O'Shea, S.Sodergren, M.Odelinus, R.Ahuja, O.Karis, M.Bassler, P.Persson, H.Siegbahn, S.Lunell and N.Martensson
Experimental evidence for sub-3-fs charge transfer from an aromatic adsorbate to a semiconductor
Nature **418**, 620 (2002).

132.Y.Wang, R.Ahuja and B.Johansson
Going to 10 TPa : The calculated Hugoniots for Cu, Ta and Mo
High Press. Research **22**, 485 (2002).

133.Y.Wang, R.Ahuja and B.Johansson
Thermodynamic Properties of MgO, Be and W : a simplified computational approach
J. Phys. C **44**, 10895 (2002).

134. Sa Li, R. Ahuja and B.Johansson
Pressure-induced phase transitions in $KNbO_3$
J. Phys. C **44**, 10873 (2002).

135.Sa Li, R. Ahuja and B.Johansson
High Pressure Theoretical Studies of Actinide Dioxides
High Press. Research **22**, 471 (2002).

136.R.Ahuja, J. M. Osorio-Guillen, C.Persson, B.Johansson, A. Ferreira da Silva, K. Järrendahl, Q. Wahab
Optical Properties Of Doped 4H-SiC
J.Appl. Phys. **91**, 2099 (2002).

137.G.Kh. Rozenberg, L.S. Dubrovinsky, M.P.Pasternak, O. Naaman, T.Le Bihan and R.Ahuja
High-pressure structural studies of hematite (Fe_2O_3)
Phys. Rev. B.**65**, 064112 (2002).

138.G.E.Grechnev, R.Ahuja, B.Johansson and O.Eriksson
Electronic Structure, magnetic and cohesive properties of $Li_xMn_2O_4$
*Phys. Rev. B***65**, 174408 (2002).

139. Jorge Osario Gullien , Yi Wang, S.Simak, B.Johansson and R.Ahuja
Bonding and elastic Properties of Supercoduting MgB_2
Solid State Commun. **123**, 257 (2002).

140.J. Souza de Almeida, A. J. da Silva, P. Norman, C. Persson, R. Ahuja and A. Ferreira da Silva
Optical properties of donor- triad -cluster in GaAs and GaN
Appl. Phys. Lett. **81**, 3158 (2002).

141.A.Grechnev, P.H.Andersson, R.Ahuja, O.Eriksson, M.Vennström and Y.Andersson
H-H interaction and structural phase transition in Ti_3SnH_x
*Phys. Rev. B***66**, 235104 (2002).

142.E.A.Smirnova, R.Ahuja, Yu.Kh.Vekilov, Y.K.Vohra, B.Johansson and I.A.Abrikosov
Effect of band filling on the pressure-induced structural transition in Mo-Re alloys
Phys. Rev. B **66**, 024110 (2002).

143.Yi Yang, R.Ahuja, O.Eriksson, B.Johansson and G.Grimval
Precise solution for H-point Phonon in Mo, Na, and Fe
J. Phys. C. : Letter to Editor **14**, L453 (2002).

144.Y. Wang, R. Ahuja and B.Johansson
Reductions of Shock-Wave Data with mean-field potential Approach
J. Appl. Phys. **92**, 6616 (2002).

145.J. -H Guo, L. Vayssieres, C. Persson, R. Ahuja, B. Johansson, and J. Nordgren
Polarization dependent soft-x-ray absorption of highly oriented ZnO microrods arrays
*J. Phys. C.***14**, 6969 (2002).

146.N.A. Dubrovinskaia, L.S. Dubrovinsky, V. Swamy and R.Ahuja
Cotunnite structureed Titanium Dioxide
High Press. Res. **22**, 391 (2002).

147.Yi Wang, Rajeev Ahuja and B.Johansson
Thermodynamic properties at the Earth's core conditions and shock-reduced Isotherm of Iron : A first-principles study
J. Phys. C **14**, 7321 (2002).

148.Y. Wang, R.Ahuja, O.Eriksson, B.Johansson and G.Grimvall
Precise Solution of H-point Oscillation : Na, Mo and Fe
J. Phys. C: Letter to Editor **14**, L453 (2002).

149.Y. Wang, R.Ahuja, M.C.Qian and B.Johansson
Quantum Mechanical Treatment of Phonon Instability : bcc Zr
J. Phys. C: Letter to Editor **14**, L695 (2002).

150.R.Ahuja, H.Arwin, A. F. da Silva, C. Persson, J. M. Osorio-Guillen, J.S. Almeida, C.M. Araujo, E. Veje, N. Veissid, C.Y. An, I. Pepe and B.Johansson
Electronic And Optical Properties Of Lead Iodide
J. Appl. Phys. **92**, 7219 (2002).

151. A.B.Belonoshko, R.Ahuja and B.Johansson
Molecular Dynamics Study of Xe
Phys. Rev. Lett. **89**, 119602 (2002).

152.A. C. de Oliveira, J. A. Freitas, Jr., W. J. Moore, A. Ferreira da Silva, I. Pepe, J. Souza de Almeida, J.M. Osorio-Guillen, R. Ahuja, C. Persson, K. Järrendahl, O. P. A. Lindquist, N. V. Edwards and Q. Wahab
TRANSMISSION AND PHOTOACOUSTIC SPECTROSCOPIES OF 4H-SiC
Materials Research **6**, 47 (2003).

153.A.C. de Oliveira, J.A.Freitas, Jr., W.J.Moore, A.Ferreira da Silva, J.Souza de Almeida, G.C.B. Braga, J. M. Osorio-Guillen, C.Persson and R.Ahuja
Photoacoustic Studies of SiC Polytypes
Materials Research **6**, 43 (2003).

154. R.Ahuja
Calculated high pressure crystal structure transformations for Phosphours
Phys. Stat. Solidi (b) **235**, 282 (2003).

155.C.Persson, R.Ahuja, J.S. Almeida, B.Johansson, C.Y. An, F.A.Ferreira, N. Souza Dantas, I. Pepe and A. F. da Silva
Optical absorption of large band-gap $Sb_xBi_{1-x}I_3$ alloys
MRS **744**, 5351 (2003).

156.A. F. da Silva, I. Pepe, H.Haratizadeh, P.O. Holtz, C.Persson, R.Ahuja, J.S. de Almeida and A. G. de Oliveria
Electronic properties of n-type $Al_xGa_{1-x}As$ alloys
MRS **744**, 8101 (2003).

157.Y. Wang, R.Ahuja and B.Johansson
LiH under high pressure and high temperature : A first principle study
Phys. Stat. Solidi (b), **235**, 470 (2003).

158.R.Ahuja
High pressure structural phase transitions in IV-VI semiconductors
Phys. Stat. Solidi (b) **235**, 341 (2003).

159.R.Ahuja, C.Persson, A. Ferreira Da Silva and B.Johansson

Optical Properties of SiGe alloys
J Appl. Phys. **93**, 3832 (2003).

160.U.Haussermann, S.I.Simak, Rajeev Ahuja and B.Johansson
Metal-nometal transition in the boron group elements
Phys. Rev. Lett. **90**, 065701 (2003).

161.G.E.Grechnev, R.Ahuja, B.Johansson and O.Eriksson
Magnetic properties of $LiMn_2O_4$ spinels
J. Mag. Mag. Mat. **258**, 287 (2003).

162.A.B.Belonoshko, R.Ahuja and B.Johansson
Stability of the body-centred cubic phase of iron in the Earth's inner core
Nature **424**, 1032 (2003).

163.Z.M.Sun, R.Ahuja, Sa Li and J.M.Schneider
Structure and bulk modulus of M_2AlC (M=Ti,V and Cr)
Appl.Phys. Lett. **83**, 899 (2003).

164.M. Colarieti-Tosti, S. I. Simak, R. Ahuja, L. Nordstrom, O. Eriksson, D. Aberg,
S. Edvardsson, and M. S. S. Brooks
Origin of magnetic anisotropy of Gd metal
Phys. Rev. Lett. **91**, 157201 (2003).

165 . P. Sharma, A. Gupta, K. V. Rao, F.J. Owens, R.Sharma,
R. Ahuja, J.M.Osorio Guillen, B.Johansson and G.A.Gehring
Ferromagnetism above room temperature in bulk and transparent thin films of Mn-doped ZnO
***Nature-Materials* 2**, 673 (2003).

166.L.S.Dubrovinsky, N.A.Dubrovinskaia, C.MaCammon, G.Kh. Rozenberg,
R.Ahuja, J.M.Osorio-Guollen, V.Dmitriev, H.P.Weber and B. Johansson
Structure of Metallic and Magnetic High Pressure Fe_3O_4 Polymorph : Experimental
and Theoretical Study
J. Phys C: Condensed Matter **15**, 7697 (2003).

167.G.Kh. Rozenberg, M.P.Pasternak, W.M.Xu,L.S.Dubrovinsky,
R.Ahuja, J.M.Osorio-Guollen, B. Johansson and T. Le Bihan
Pressure-induced Structural Transformations in the MottInsulator FeI_2
Phys. Rev. B **68**, 064105 (2003).

168.G.E.Grechnev, R.Ahuja and O.Eriksson
High Pressure Magnetic Susceptibility of Iron and its Implications to Seismic
Anisotropy of Earth,s Inner core
*Phys. Rev. B***68**, 064414 (2003).

169.A. Srivastava, R.K. Singh, R.Ahuja and B.Johansson,
High-pressure phase transitions in semimagnetic semiconductor I: $Pb_{1-x}Mn_xS$

Phys. Status sol.(b) **237**, 448 (2003).

170. Z.M.Sun, R.Ahuja and J.M.Schneider
Theoretical investigation of solubility in $M_xM'_{2-x}AlC$ (M=Ti,V and Cr)
Phys. Rev. B **68**, 224112 (2003).

171.M.Mattesini, R.Ahuja and B.Johansson
Cubic Hf_3N_4 and Zr_3N_4 : A class of hard materials
Phys. Rev. B **68**, 184108 (2003).

172.Sa Li, R.Ahuja, Y.Wang and B.Johansson
Crystallographic structure of $PbWO_4$
High Press. Res. **23**, 343 (2003).

173.A.Grechnev, R.Ahuja and O.Eriksson
Balanced crystal orbital overlap population (BCOOP)-a tool for analysing chemical bonds in solids
J. Phys. C: Condensed Matter. **15**, 7751 (2003).

174.G.E. Grechnev, R. Ahuja and O. Eriksson,
Magnetic properties of HCP iron and seismic anisotropy of the Earth's core
High Pressure Phys. and Technology **13**, 14 (2003).

175.J.Kollar, L.Vitos, J.M.Osorio Guillen and R.Ahuja
Calculation of surface stress for fcc transition metals
Phys. Rev. B **68**, 245417 (2003).

176.A. FERREIRA DA SILVA, C. PERSSON, P. NORMAN, J. SOUZA DE ALMEIDA, A. J. DA SILVA AND R. AHUJA
Evidence of Donor-Triad Cluster in GaN and GaAs
Phantoms Newsletter, October 2003, Issue **12/13**.

177.M. C. ANDRADE, C. S. S. BRASIL, I. PEPE, A FERREIRA DA SILVA, N. S.DANTAS, D. G. F. DAVID, C. Y. AN, N. VEISSID, L. N. CHRISTENSEN, E. VEJE, H. ARVIN, C. PERSSON AND R. AHUJA
Optical Properties of Large-Bandgap PbI_2 and $SbBiI_3$
Annals of Optics **5**, 100 (2003).

178.A.B.Belonoshko, R.Ahuja and B.Johansson
Body-centred cubic iron in the Earth's inner core
Solid State Physics (Allied Publishers Pvt. Ltd., New Delhi, India) **46**, 933 (2003).

179.R.Ahuja, L.Dubrovinsky, N.Dubrovinskaia, J.M.Osorio Guillen, M.Mattesini, B.Johansson and T. Le Bihan
Titanium metal at high pressure : Synchrotron experiments and *ab initio* calculations
Phys. Rev.B **69**, 184102 (2004).

180.J. M. Osorio-Guillen, R.Ahuja, B.Holm and B.Johansson
A theoretical study of olivine $LiMPO_4$ (M= Fe and Co) cathodes
Solid State Ionics **167**, 221 (2004).

181.R.Ahuja, J. M. Osorio-Guillen, J.Almeida B.Holm, W.Y.Ching and B.Johansson
Electronic and optical properties of γ-Al_2O_3 from *ab initio* theory
J. Phys. Condens. Matter **16**, 2891 (2004).

182.A.B.Belonosko, Sa Li, R.Ahuja and B.Johansson
High-pressure crystal structure studies of Fe, Ru and Os
J. Phys. Chem. Solids **65**, 1565 (2004).

183.Y. Wang, R.Ahuja and B.Johansson
Mean-Field Potential Approach to the Quasiharmonic Theory of Solids
Int. J. of Quantum Chem. **96**, 501 (2004).

184. M. Agaker, J.Soderstrom, T Kaambre, C.Glover, L.Gridneva, T.Schmitt,
A.Augsutsson M.Mattesini, R.Ahuja and J.E.Rubensson
Resonant inelastic soft x-ray scattering at hollow lithium state in solid LiCl
Phys. Rev. Lett., **93**, 016404 (2004).

185.M.Tosti, M.I.Katsnelsen, M.Mattesini, S.I.Simak, R.Ahuja, B.Johansson,
C.Dallera and O.Eriksson
First Principles theory of intermediate valence *f*-electron systems
Phys. Rev. Lett., **93**, 096403 (2004).

186.A. Grechnev, S.Li, R.Ahuja, O.Eriksson, U.Jansson and O.Wilhelmsson
A new nanolayered material, Nb_3SiC_2, predicted from First Principles Theory
Appl. Phys. Lett. **85**, 3071 (2004).

187.Y. Wang, R.Ahuja and B.Johansson
A Model for Phase Coexistence in Phase Transitions
Int. J. of Quantum Chem. **97**, 961 (2004).

188.J.S.Tse, Z. Li, K.Uehara, Y.Ma and R.Ahuja
Electron-Phonon coupling in high pressure Nb
Phys. Rev. B **69**, 132101 (2004).

189.Z.Sun, Sa Li, R.Ahuja and J.M.Schneider
Calculated elastic properties of M_2AlC (M=Ti,V,Cr,Nb and Ta)
Solid State Commun. **129**, 589 (2004).

190.T. Schmitt, L.-C. Duda, M. Matsubara, M. Mattesini, M. Klemm, A. Augustsson,
J.-H. Guo, T. Uozumi, S. Horn, R. Ahuja, A. Kotani, and J. Nordgren
Electronic structure studies of V_6O_{13} by soft x-ray emission spectroscopy:
Band-like and excitonic vanadium states
Phys. Rev. B **69**, 125103 (2004).

191. E.I.Isaev, A.I.Lichtenstein, Yu.Kh.Vekilov, E.A.Smirnova, I.A.Abrikosov, S.I.Simak, R.Ahuja and B.Johansson
Ab initio phonon calculations for $L1_2$ Ni_3Al and B2 NiAl
Solid State Commun. **129**, 809 (2004).

192.J.M.Schneider, Z.Sun, R.Mertens, F.Uestel and R.Ahuja
Ab initio calculations and experimental determination of the structure of Cr_2AlC
Solid State Commun. **130**, 445 (2004).

193.Sa Li, R.Ahuja and B.Johansson
Wolframite : the post-fergusonite phase in $YLiF_4$
J.Phys.C. Condensed Matter **16**, S983 (2004).

194.N.Skorodumova, R.Ahuja and B.Johansson
Influence of hydrogen on the stability of iron phases under pressure
Geophysical Research Lett. **31**, L08601 (2004).

195. M.Mattesini, J.Almedida, L.Dubrovinsky, N.Dubrovinkaia, B.Johansson and R.Ahuja
Cubic TiO_2 as a potential light absorber in solar-energy conversion
Phys. Rev. B **70**, 115101 (2004).

196.P.Souvatzis, J.M.Osorio Guillen, R.Ahuja, A.Grechnev and O.Eriksson
Elastic properties of $Mg_{1-x}Al_xB_2$ from first principles theory
J.Phys.:Condens. Matter **16**, 5241 (2004).

197.P.Souvatzis, P.Mohn, M.I.Katsnelson, S.Simak, R.Ahuja and O.Eriksson
First-principles prediction of superelastic transition metal alloys
Phys. Rev. B **70**, 012201 (2004).

198.A.Ferreria, I.Pepe, B.E.Sernelius, C.Persson, R.Ahuja, J.P.Souza and Y.Wang
Electrical Resistivity of acceptor carbon in GaAs
J. Appl. Phys. **95,** 2532 (2004).

199.A.Ferreria, I.Pepe, J.Almeida, C.Moyses, C.Persson, R.Ahuja, B.Johansson and J.H.Guo
Optical properties of Oxide compounds PbO, SnO_2 and TiO_2
Physica Scripta **T109**, 180 (2004).

200.T.Andersen and R.Ahuja
Linear and nonlinear semiclassical optics beyond the electric dipole approximation
Physica Scripta **T109**, 106 (2004).

201.P.Finkel, J.D.Hettinger, S.E.Lofland, K.Harrell, A.Ganguly, M.W.Barsoum Z.Sun, Sa Li and R.Ahuja
Low temperature Elastic, electronic and transport properties of
$Ti_3Si_xGe_{1-x}C_2$ solid solutions

Phys. Rev. B **70**, 085104 (2004).

202.Z.Sun, D.Music, R.Ahuja, Sa Li and J.M.Schneider
Bonding and classification of nanolayered ternary carbides
Phys. Rev. B **70**, 092102 (2004).

203. C.M.Araujo, A.F.da Silva, C. Persson, R.Ahuja and E.D.A.E. Silva
Spin dependent conductance in nonmagnetic InGaAs asymmetric double barrier devices
B. J. Phys. **34**, 632 (2004).

204.M. Marques, J.Osorio, R.Ahuja, M.Florez and J.M.Recio
Pressure effects on the structure and vibrations of C_3N_4
*Phys. Rev. B***70**, 104114 (2004).

205.J.P.Palmquist, Sa Li, P.O.A.Persson, J.Emmerlich, O.Wilelmsson, H.Hogberg
M.I.Katsnelson, B.Johansson, R.Ahuja, O.Eriksson, L.Hultman and U.Jansson
New MAX phases in the Ti-Si-C system studied by thin film synthesis and
ab initio calculations
*Phys. Rev. B***70**, 165401 (2004).

206.M.Colarieti-Tosti, S.Simak, R.Ahuja, L.Nordstrom,O.Eriksson,
and M.S.S. Brooks
Theory of the Magnetic Anisotropy of Gd Metal
*Journal of Mag. and Mag. Mater. 2***72**, E201(2004).

207.A FERREIRA DA SILVA, I. PEPE, C.S. S. BRASIL, D. G. F. DAVID,
E. F. DA SILVA,JR, J. S. DE ALMEIDA, C. MOYSES ARAUJO, C. PERSSON,
R. AHUJA AND T. LINDGREN
Electronic and Optical Properties of Rutile Titanium Dioxide
Physica Status Solidi (c)1 **S2**, 241 (2004).

208.J. M. Osorio-Guillen, R.Ahuja and B.Johansson
Structural Phase Transition in Heavy Alkali Metals Under Pressure
Chem. Phys. Chem. **5,** 1411 (2004).

209.M.Stromme, R.Ahuja and G.A.Niklasson
A new probe of the electronic structure of Amorphous materials
Phys. Rev. Lett. **93** 206403 (2004).

210.C.L. Dong, C. Persson, L.Vayssieres, A.Augustsson, T.Schmitt,
M.Matesini, R.Ahuja, C.L.Chang and J.H.Guo
Electronic structure of nanostructured ZnO from X-ray absorption
and emission spectroscopy and LDA calculations
Phys. Rev. ***B*****70**, 195325 (2004).

211.G.E. Grechnev, R.Ahuja, J. Guo and O.Eriksson
Electronic structure and optical spectra of novel rechargeable lithium batteries

SPIE, Int. Soc. Optical Eng. **5507,** 35 (2004).

212.M.Mattesini, J.Almedida, L.Dubrovinsky, N.Dubrovinkaia, B.Johansson and R.Ahuja
High-pressure and high-temperature synthesis of the cubic TiO_2 polymorph
*Phys. Rev. B***70**, 212101 (2004).

213. C. Moyses Araujo, A. Ferreira da Silva and R. Ahuja
Structural phase transition in ErH_3
Physica Status Solidi (b) **241**, 3219 (2004).

214.R.Ahuja, A.B.Belonoshko, B.Johansson and A.Osiptsov
Inertial Phase Segregation in rotating self-gravitating media
Fluid Dynamics, **39***,(*2004)

215.R. R. ROSA, A. FERREIRA DA SILVA, R. C. BRITO, I. PEPE,
L. S. ROMAN. M.P.M.A BARONI, F. M. RAMOS, R. AHUJA AND C. PERSSON
Structural Flyby Characterization of Nanoporosity
Physica Status Solidi (c) **1,** S277 (2004).

216.Y.Ma, J.S.Tse, D.Klug and R.Ahuja
High Pressure Superconducting Phase of Boron
Phys. Rev. B**70**, 214107 (2004).

217.W.Luo, S.F.Wang, Z.C.Wang, Y.Wang, R.Ahuja, B.Johansson, H.Y.Chen, J.Liu and Z.T.Zou
High pressure studies on polycrystalline brookite-type TiO_2
Solid State Commun. **133**, 49 (2005).

218.C.M.Araujo and R.Ahuja
Electronic and optical properties of pressure induced phases of MgH_2
J.Alloys and Compounds **404**, 220 (2005).

219.S. A TOMAS, S. STOLIK, R. PALOMINO, R. LOZADA, C. PERSSON,
R. AHUJA, T. LINDGREN, A FERREIRA DA SILVA AND I. PEPE
Optical Properties of Rhodamine 6G-Doped TiO_2 Sol-Gel Films
Journal de Phisique IV **125**, 415 (2005).

220.N. G. ASTRATH, A. C. BENTO, M. L. BAESSO, A FERREIRA DA SILVA,
I.PEPE, R. AHUJA, C. PERSSON, S. ZHAO AND C.-G. GRANQVIST
Thermal Lens and Photoacoustic Spectroscopy to Determine the Thermal
and Optical Properties in Bulk and Thin Film Semiconductors
Journal de Phisique IV **125**, 181 (2005).

221.M. V. CONCEICAO, O. NAKAMURA, A FERREIRA DA SILVA,
L. V. SANTOS, V. J. TRAVA-AIROLDI AND L. S. ROMAN

Photoacoustic Investigations of Optical Absorption, Energy Gap, and
Thermal Diffusivity of Porous Diamond – Like- Carbon Films
Journal de Phisique IV **125**, 293 (2005).

222.A Ferreira da Silva, N. Souza Dantas, J. S. de Almeida , R. Ahuja and C. Persson,
Electronic and Optical of Wurtzite and Zinc-Blende TlN and AlN
J. Cryst. Growth **281,** 151 (2005).

223. Y.Wang, Z.K.Liu, L,Q.Chen, L.Burakovsky, D.L.Preston, W.Luo, B.Johansson
and R.Ahuja
Mean-field Potential Calculations of Shock-compressed Porous Carbon
*Phys. Rev. B***71**, 054110 (2005).

224.L.Huang, N. Skorodumvoa, A.Belonoshko, B.Johansson and R.Ahuja
Carbon in iron under high pressure
GeoPhys. Res. Letters. **32***,* L21314 (2005).

225.N. Skorodumvoa, L.Huang, A.Belonoshko, B.Johansson and R.Ahuja
New high pressure phase in $MgCO_3$
American Minerologist **90***,* 1008 (2005).

226.A.B.Belonshko N. Skorodumvoa, A.Rosengren, R.Ahuja, B.Johansson,
L.Burakovsky and D.L.Preston
High Pressure Melting of $MgSiO_3$
Phys. Rev.. Letters. **94**, 195701 (2005).

227. M.Magnuson, J.P.Palmquist, M.Mattesini, Sa Li, R.Ahuja J.Emmerlich, O.Wilelmsson,
O.Eriksson, P.Eklund, H.Hogberg, L.Hultman and U.Jansson
Electronic structure of the MAX-phases Ti_3AC_2 (A=Al,Si,Ge)
investigated by soft x-ray absorption and emission spectroscopies
*Phys. Rev. B***72**, 245101 (2005).

228.Denis Music, R.Ahuja and J.M.Schneider
Theoretical study of nitrogen vacancies in Ti_4AlN_3
Appl. Phys. Lett. **86**, 031911 (2005).

229. S.A.Boye, P.Lazor and R.Ahuja
Magnetoresistance and Hall Effect Measurements of Ni Thin Films
J. Appl. Phys. **97**, 083902 (2005).

230. S. A.Boye, P.Lazor and R.Ahuja
Magnetoresistance and Hall Effect Measurements of Ni up to 6 GPa
J.Mag. Mag. Mat. ***294,*** *347 (2005)*

231. A Ferreira da Silva, N. Souza Dantas, E. F. Da Silva Jr, I. Pepe, M. O. Torres,
C. Persson, T. Lindgren, J. Souza de Almeida and R. Ahuja.
Electronic and Optical Properties of TiO_2

AIP Conference Proceedings **772**, 175 (2005).

232. A Ferreira da Silva, N. Souza Dantas, R. Ahuja, I. Pepe, E. F. da Silva Jr., O Nur , M. Willander and C. Persson ,
Linear Optial Response of $Si_{1-x}Ge_x$ Compounds ,
SPIE, **5732**, 556 (2005).

233. Sa Li and R.Ahuja
Electronic, Elastic and Optical properties of Y_2O_2S
J. Appl. Phys. **97***,* 103711 (2005)

234. C.M.Araujo, R.Ahuja, J.M.O.Guillen and P.Jena
Role of Titanium in Hydrogen Desorption in Crystalline Sodium alanate
Appl. Phys. Lett **86***,* 251913 (2005).

235.Z.Sun, D.Music, R.Ahuja and J.M.Schneider
Ab initio investigation on M_2AlN (M=Ti, V, Cr)
J. Phys. C : Condens. Matt.(Letter to Editor) **17**, L15 (2005).

236.Z.Sun, D.Music, R.Ahuja and J.M.Schneider
Theoretical investigation of bonding and elastic properties of nanolayered Ternary nitrides
*Phys. Rev. B.***71**, 193402 (2005).

237. C.Moyses Araujo, S.Li, R.Ahuja and P.Jena
Vacancy Mediated Hydrogen Desorption in Sodium-Alanate
*Phys. Rev. B***72**, 165101 (2005).

238. S. Heathman, R. G. Haire, T. Le Bihan, A. Lindbaum, M. Idiri, P. Normile, S. Li, R. Ahuja, B. Johansson, and G. H. Lander,
A new high-pressure structure in curium linked to magnetism,
Science **309**, 110 (2005).

239. C. Moysés Araújo, R. Ahuja, A. V. Talyzin, and B. Sundqvist,
Pressure-induced structural phase transition in $NaBH_4$
Phys. Rev. B. B **72**, 054125 (2005).

240. Z.Sun, D.Music, R.Ahuja, and J.M.Schneider,
Electronic origin of the shear property in M_2AX,
*J.Phys. C***17**, 7169 (2005).

241. S.K.Kwon, Z.Nabi, K.Kadas, L.Vitos, J.Kollar, B.Johansson and R.Ahuja,
Surface Energy and Stress Release by Layer Relaxation,
*Phys. Rev. B***72**, 235423 (2005).

242. E.I.Isaev, R.Ahuja, S.I.Simak, A.I.Lichtenstein, Y.K.Vekilov, B.Johansson

and I.A.Abrikosov
Anomalously enhanced superconductivity and ab initio lattice dynamics in transition Metel carbides and nitrides
Phys. Rev. B **72**, 064515 (2005).

243. A.Augustsson, G.V.Zhuang, S.M.Butorin, J.M.Osorio-Guillen, C.L.Dong, R.Ahuja, C.L.Chang, P.N.Ross, J.Nordgren and J.H.Guo,
Electronic structure of phospho-olivines LixFePO4(x=0.1) from soft-x-ray absorption and Emission spectroscopy
J. Chem. Phys. **123**, 184717 (2005).

244. C. Moysés Araújo, S. Lebègue, O. Eriksson, B. Arnaud, M.Alouani and R.Ahuja
Electronic and optical properties of MgH2: a first-principle GW investigation,
J. Appl. Phys. **98**, 096106 (2005).

245. (a) N. Dubrovinskaia, L. Dubrovinsky, I. Kantor, W. A. Crichton, V. Dmitriev,V. Prakapenka, G. Shen, L. Vitos, R. Ahuja, B. Johansson, and I.A.Abrikosov
Beating the Miscibility Barrier between Iron Group Elements and Magnesium by High-Pressure Alloying
*Phys. Rev. Lett.***95,** 245502 (2005).

245.(b) One of the figure (Fig.3) of above paper has been appeared on the cover page of *Phys. Rev. Lett* **95 (Nr. 24 Articles published 3 December - 9 December 2005).**
Title of the cover page was ´´ Electrically and laser-heated diamond anvil cell is used to demonstrate that high pressure promotes solubility of magnesium in iron.

246. C.M. Araujo, S.Li, R.Ahuja and P.Jena,
Mechanisms for hydrogen desorption in sodium alanate,
ACS division of Fuel Chemistry **50,** 22 (2005).

247. Z.Nabi, L.Vitos, B.Johansson and R.Ahuja
Ab initio calculations of elastic properties of solid He under pressure,
*Phys. Rev. B***72**, 172102 (2005).

248. S. Li, P.Jena, C.Moyses Araujo and R.Ahuja
Electronic structure and hydrogen desorption in $NaAlH_4$
Mater. Res. Soc. Symp. Proc. **837,** 29 (2005).

249. C.Moyses Araujo, S.Li, R.Ahuja and P.Jena
Vacancy Mediated Hydrogen Desorption in Sodium-Alanate
Papers of the American Chemical Society 229 : U852 (2005).

250.C.L. Dong, M.Mattesini, A.Augustsson, X.G.Wen, W.X. Zhang, S.H.Yang C.Persson, R.Ahuja, J.Luning, C.L.Chang and J.H.Guo
Electronic structure and surface structure of Cu_2S nanorods from polarization

dependent X-ray absorption spectroscopy
J. of Electron Spect. And Related Phenomena, **151,** 64 (2006).

251.L.Vitos, B.Kope, R.Ahuja, J.Kollar, G.Grimvall and B.Johansson
Phase seperation in Ca-bearing minerals-Relation to seismic discontinuities
Phys. Earth and Planetary Interiors **156,** 108 (2006).

252.Sa Li, R.Ahuja and B.Johansson
Elastic and optical properties of the high pressure hydrous phase δ-AlOOH
Solid State Comun. **137,** 101 (2006).

253.I.Kantor, L.Dubrovinsky, C.McCammon, A.Kantor, S.Pascarelli, G.Aquilanti, W.Crichton, M.Mattesini, R.Ahuja, J.Almeida and V.Urusov
Rhombohedral distortion of $Mg_{0.8}Fe_{0.2}O$ ferropericlase at high pressures
Phys. Chem. Minerals **33,** 35 (2006*).*

254.Z.Sun, J.Zhou, D.Music, R.Ahuja, Y.Zhou and J.M.Schneider
The anomalous strength of Ti_3SiC_2 at high temperatures induced by phase transformation
Scripta Metallurgica **54**, 105 (2006).

255. Z.Sun, D.Music, R.Ahuja, and J.M.Schneider,
Ab initio study of the chemical bonding and mechanical properties of Li_2SiZn,
J. Appl. Phys. **99**, 053509 (2006).

256. C.M.Fang, R.Ahuja, O.Eriksson, U.Jansson, O.Wilhelmsson and L.Hultman,
General trend of the Mechanical properties of the Ternary carbides
M_3SiC_2 (M=transition metal),
*Phys. Rev. B***74**, 054106 (2006).

257. M. P. M. A. Baroni, R. R. Rosa, A. Ferreira da Silva, I. Pepe, L. S. Roman, F. M. Ramos, R. Ahuja, C. Persson and E. Veje
Modeling and gradient pattern analysis of irregular SFM structures of porous silicon
Microelectronics Journal **37**, 290 (2006).

258.A.Yu. kuznetsov, J. S. de Almeida, L.Dubrovinsky, R.Ahuja, S.K.Kwon, I.Kantor, A.Kantor and N.Guignot
High Pressure synthesis and physical properties of a new orthorhombic phase of chromium dioxide,
J. Appl. Phys. **99,** 053909 (2006).

259. Z.Sun, J.Zhou and R.Ahuja,
Structure of Phase Change materials for data storage
Phys. Rev. Lett. **96**, 055507 (2006).

260. K.Kadas, Z.Nabi, S.K.Kwon, L.Vitos, R.Ahuja, B.Johansson and J.Kollar,
Surface relaxation and surface stress of 4d transition metals
Surface Science **600,** 395 (2006).

261. L.Huang, L.Vitos, S.K.Kwon, B.Johansson and R.Ahuja,
Thermoelastic properties of random alloys from first-principles theory
*Phys. Rev.B***73,** 104203 (2006).

262. C.M.Fang and R.Ahuja,
Structure and Stability of ABO_3 orthorhombic perovskites at earth's mantle
Conditions from first principles theory,
Phys. Earth and Planetary Interiors **157,** 1 (2006)

263. J. Almeida and R.Ahuja
Electronic and optical properties of RuO_2 and IrO_2,
*Phys. Rev. B***73,** 165102 (2006).

264. D.Music, Z.Sun, R.Ahuja and J.M.Schneider,
Coupling in nanolaminated ternary carbides studied by theoretical means :
influence of electronic potential approximations,
*Phys. Rev.B***73,** 134117 (2006).

265. L.S.Roman, R.Valaski, C.D.Canestraro, E.C.S.Magalhaes, C.Persson, R.Ahuja
E.F. da Silva Jr., I. Pepe and A.Ferreira da Silva
Optical band-edge absorption of oxide compound SnO_2
Applied Surface Science **252,** 5361 (2006).

266. A.Ferreira da Silva, I.Pepe, James L. Gole, S.A.Tomas, R.Palomino,
W.M. dc Azevedo, E.F. da Silva Jr., R.Ahuja and C.Persson,
Optical properties of in situ doped and undoped titania nanocatalysts and doped
Titania sol-gel nanofilms,
Applied Surface Science **252,** 5365 (2006).

267. Z.Sun and R.Ahuja,
Ab initio study of Cr_2AlC (0001) surface
Appl. Phys. Lett. **88**, 161913 (2006).

268. R.Ahuja, Z.Sun and W.Luo
Ab initio investigation on the phase stability of Ti_3SiC_2, $Ti_3Si_{0.5}Ge_{0.5}C_2$ and
Ti_3GeC_2 at high pressures
High Pressure Research **26,** 127 (2006).

269. S.Li, R.Ahuja and B.Johansson,
Phase transitions in $Am_{0.5}Cm_{0.5}$ binary alloy,
Mater. Res. Soc. Symp. Proc. **893**, 233 (2006).

270. R.Ahuja S. Li and B.Johansson,
High Pressure structural transitions in Cm metal,
Mater. Res. Soc. Symp. Proc. **893**, 247 (2006).

271. G.A. Niklasson, L.Berggren, Anna K. Jonsson, R.Ahuja,
N.V.Skorodumova, J.Backholm and M.Stromme,
Electrochemical studies of the electron states of disordered electrochromic
Oxides,
Solar Energy Materials & Solar Cells **90**, 385 (2006).

272. O. Wilhelmsson, J.-P. Palmquist, E. Lewin, J. Emmerlich, P. Eklund,
P.O.Å. Persson, H. Högberg, S. Li, R. Ahuja, O. Eriksson, L. Hultman and U. Jansson
Deposition and Characterization of Ternary Thin Films within the Ti-Al-C System
by dc Magnetron Sputtering,
J. Crystal Growth **291,** 290 (2006).

273. G.A. Niklasson, R.Ahuja and M.Stromme,
Electronic states in intercalation materials studied by electrochemical techniques,
*Modern Physics Letters B***20,** 863 (2006).

274. A.Gupta, F.J.Owens, K.V.Rao, Z. Iqbal, J.M.Osorio Guillen and R.Ahuja
High Temperature Ferromagnetism in Gallium Phosphide Doped with copper,
*Phys. Rev. B.***74,** 224449 (2006).

275. M.L.F. Koci, E.M.Bringa, D.S.Ivanov, J.Hawreliak, J.M.Naney, A.Higginbotham,
L.V. Zhigilei, A.B.Belonoshko, B.A.Remington and R.Ahuja
Simulation of shock-induced melting of Ni using molecular dynamics coupled
to a two temperature model,
*Phys. Rev. B***74,** 012101 (2006).

276. L.Koci, A.B.Belonoshko and R.Ahuja,
Molecular dynamics calculations of liquid iron properties and adiabatic Temperature
Gradient in the Earth's outer core,
Geophysical Journal International **168,** 890 (2007).

277. F. Cricchio, A.B.Belonoshko, L.Burakovsky, D.L.Preston and R.Ahuja
High Pressure melting of Lead,
*Phys. Rev. B***73***,* 140103 (2006).

278. C.Dallera, O.Wessely, M.Tosti, O.Eriksson, R.Ahuja, B.Johansson, M.I.Kastsnelson,
E.Annese, J.-P.Rueff, G.Vanko, L.Braicovich and M.Grioni,
Understanding mixed valent materials : dynamical core hole screening in x-ray
High pressure spectroscopy,
Phys. Rev. B **74,** 081101 (2006).

279. L.Huang, A.L.Rosa and R.Ahuja,
Ferromagentism in (Zn,Cu)O from first principles theory,
Phys. Rev. B74, 075206 (2006).

280. Y.Wang, Z.K.Liu, L.Q.Chen, L.Burakovsky and R.Ahuja
First-principles calculation of MgO : Phonon theory vs mean field potential approach,
J. Appl. Phys. **100,** 023533 (2006).

281. S.Li, P.Jena and R.Ahuja,
Effect of Ti and metal vacancies on the electronic structure, stability and
Dehydrogenation of Na_3AlH_6 : Supercell band structure formalism and gradient
Corrected density functional theory
Phys. Rev. B **73,** 214107 (2006).

282. B.Johansson, S.Li, E. Isaev and R.Ahuja
Theoretical study of protactinium at high pressure,
Mater. Res. Soc. Symp. Proc. **893,** 255 (2006).

283. C Persson, A Ferreira da Silva , C L Dong , L Vayssieres , A Augustsson, T Schmitt,
M Mattesini, R Ahuja, J Nordgren, C L Chang and J H Guo ,
X-Ray absorption and emission spectroscopy of ZnO nanoparticle and highly oriented
ZnO microrod arrays,
Microelectronics Journal **37,** 686 (2006).

284. P.Larsson, R.Ahuja, A.Nyten and J.O.Thomas,
An ab initio study of the Li-ion battery cathode material Li_2FeSiO_4
Electrochemistry Communications **8,** 797 (2006).

285. D. W. Shin, C.Dong, M.Mattesini, A.Augustsson, S.Mao, C.L.Chang,
C.Persson, R.Ahuja, J.Nordgren, S X. Wang and J.H.Guo
Size dependence of the electronic structure of copper nanoclusters in SiC matrix
Chemical Physics Letters **422**, 543 (2006).

286. D.Music, R.Ahuja and J.M.Schneider
Electronic structure and lattice dynamics of $CaPd_3B$ studied by first principles
Methods
Physics Letters A **356**, 251 (2006).

287.S.Li, P.Jena and R.Ahuja,
Dehydrogenation Mechanism in Catalyst-activated MgH_2
*Phys. Rev. B*74, 132106 (2006).

288. S.Lebegue, C.Moyses Arujo, O.Eriksson, B.Arnaud, M.Alouani and R.Ahuja
Quasi particle and optical properties of BeH_2
J.Phys. : Condensed Matter **19**, 036223 (2007).

289. A.B.Belonoshko, S.D.Irarrazabal, A.Rosengren, R.Ahuja, B.Johansson,
S.I.Simak, L.Burakovsky and D.L.Preston,
Xe melting : Density functional theory vs. diamond anvil cell experiment
Phys. Rev. B. **74**, 054114 (2006).

290. A.S.Mikhaylushkin, N.V.Skorodumova, R.Ahuja and B.Johansson,
Structural and magnetic properties of FeH_x (x=0.25, 0.50, 0.75),
AIP Conference Proceedings Edited by G.Rao Myneni and B.Hjörvarsson,
Volume **837**, 161 (2006).

291. M. Emilsson, C.Moyses Araujo and R.Ahuja,
Hydrogen Desorption in High Pressure Phases of MgH_2 : a Density Functional Based Study,
AIP Conference Proceedings Edited by G.Rao Myneni and B.Hjörvarsson,
Volume **837**, 168 (2006).

292. D.Music, Z.Sun, R.Ahuja and J.M.Schneider,
Electronic structure of M2AlC (0001) surfaces (M=Ti,V,Cr)
J.Phys. : Condensed Matter **18,** 8877 (2006).

293. J.Almeida and R.Ahuja,
Tuning structural, electronic and optical properties of $Be_xZn_{1-x}Te$
Appl. Phys. Lett. ***89***, 061913 (2006).

294. L.Koci, A.B.Belonoshko and R.Ahuja,
Molecular dynamics study of liquid iron under high pressure and high temperature
Phys. Rev. B. **73**, 224113 (2006).

295. A.Grigoriev, N.V.Skorodumova, S.I.Simak, G.Wendin, B.Johansson and R.Ahuja,
Electron transport in stretched monoatomic gold wires
Phys. Rev. Lett. **97**, 236807 (2006).

296. M. Agaker, T. Kaambre, C.Glover, T.Schmitt, M.Mattesini, R.Ahuja,
J.Soderstrom, and J.E.Rubensson
Resonant inelastic soft x-ray scattering at double core excitations in solid LiCl
*Phys. Rev. B***73**, 245111 (2006).

297. M.Magnuson, M.Mattesini, O.Wilelmsson, J.Emmerlich, Sa Li, R.Ahuja,
L.Hultman, O.Eriksson, and U.Jansson,
Electronic structure and chemical bonding in Ti_4SiC_3 investigated by
soft x-ray emission spectroscopy and first principles theory
*Phys. Rev. B***74**, 205102 (2006).

298. M.Magnuson, O.Wilelmsson, J.P. Palmquist, U.Jansson M.Mattesini, Sa Li,
R.Ahuja andO.Eriksson,
Electronic structure and chemical bonding in Ti_2AlC investigated by
soft x-ray emission spectroscopy
*Phys. Rev. B***74**, 195108 (2006).

299. A.Gupta, F.J.Owens, K.V.Rao, Z. Iqbal, J.M.O.Gullien and R.Ahuja

High-temperature ferromagnetism in Cu-doped GaP by SQUID magnetometry
and ferromagnetic resonance measurements
*Phys. Rev. B***74**, 224449 (2006).

300. R.Ahuja S. Li, W.Luo and B.Johansson,
High Pressure structural transitions in Cm and AmCm binary alloys,
High Pressure Research **26**, 377 (2006).

301. R.Ahuja
Materials Design from ab initio calculations : Nanolayered MAX phases,
Proceedings of DAE-BRNS International Symposium on Materials Chemistry,
Editors; S.R.Bharadwaj, S.K.Kulshreshta et. al.(Mumbai, India)
Page :4-8 (2006).

302 (a). Z.Sun, J.Zhou and R.Ahuja,
Unique melting behaviour in Phase Change materials for rewritable data storage
Phys. Rev. Lett. **98,** 055505 (2007).

302(b). Above paper is selected as **RESEARCH HIGHLIGHTS in NATURE**.
Title of the highlight was ***How memories melt away***
Nature **445,** 687 (2007).

303. Y.Ding, R.Ahuja, J.Shu, P.Chow, W.Luo and H.K.Mao
Phase Transition of Vanadium at 69 GPa
Phys. Rev. Lett. **98**, 085502 (2007).

304. S. Heathman, R. G. Haire, T. Le Bihan, R.Ahuja S. Li, W.Luo and B.Johansson,
The Unique high pressure behaviour of curium probed further using alloys
J. Alloys and Compounds **444,** 138 (2007).

305. C.M.Fang, R.Ahuja and O.Eriksson,
Prediction of new MX phases, $V_{N+1}SiC_N$ (N=1,2), from first principles theory
J.Appl. Phys. **101,** 013511 (2007).

306. D.Music, Z.Sun, R.Ahuja and J.M.Schneider,
Surface energy of M2AC(0001) determined by ab initio calculations
(M=Ti,V,Cr; A=Al,Ga,Ge)
Surface Science **601**, 896 (2007).

307. L. Koci, R.Ahuja, A.B.Belonoshko and B.Johansson,
Study of the high pressure helium phase diagram using molecular dynamics
J.Phys. : Condensed Matter **19,** 016206 (2007).

308. W.Luo and R.Ahuja,
Ab initio prediction of high-pressure structural phase transition in BaH_2
J. Alloys and Compounds **446-447,** 405 (2007).

309. A.Blomqvist, C.M.Araujo, P.Jena and R.Ahuja
Dehydrogenation from 3d-transition metal doped $NaAlH_4$: Prediction of Catalysts
Appl. Phys. Lett. **90**, 141904 (2007).

310. A.Gupta, F.J.Owens, K.V.Rao, Z. Iqbal, J.M.O.Gullien and R.Ahuja
Unusual room temperature ferromagnetism in bulk sintered GaP doped with Copper
IEEE TRANSACTIONS ON MAGNETICS **43,** 3043 (2007).

311. J-H Guo, A. Gupta, P. Sharma, K. V. Rao, M.A.Marcus, C. L. Dong, J. M. O. Guillen, S. M. Butorin, M.Mattesini, P. A.Glans, K. E. Smith, C. L. Chang and R. Ahuja
X-ray spectroscopic study of the charge state and local ordering of room-temperature Ferromagnetic Mn-doped ZnO
J. Phys.: Condens. Matter **19,** 172202 (2007).

312. D.Y.Kim, J.Almeida, L.Koci and R.Ahuja
Dynamical Stability of the Hardest known oxide and Novel cubic Solar Material : TiO_2
Appl. Phys. Lett. **90,** 171903 (2007).

313. E.Isaev, N.V.Skorodumova, R.Ahuja, and B.Johansson
Dynamical Stability of Fe-H in the Earth's Mantle and Core Regions
PNAS (the Proceedings of the National Academy of Sciences,USA) **104,** 9168 (2007).

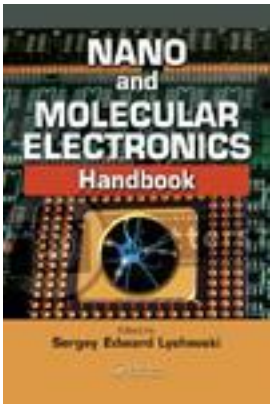
314. W.Luo and R.Ahuja
Magnetic $Fe_{n+1}AC_n$ (n = 1, 2, 3, and A = Al, Si, Ge) phases: From *ab initio* theory
J. Phys.: Condens. Matter. **20,** 064217 (2008).

315. S.Gowtham, R.H. Scheicher, R.Ahuja, R. Pandey, S.P. Karna
Physisorption of nucleobases on graphene: Density-functional calculations
Phys. Rev. B **76**, 033401 (2007).

316.P. Larsson, J. A.Larsson, R.Ahuja, F.Ding, B. I. Yakobson, H. Duan, A.Rosén, and K. Bolton
Calculating carbon nanotube–catalyst adhesion strengths
Phys. Rev. B **75**, 115419 (2007).

317. L.Koci, R.Ahuja and A.B.Belonoshko
Ab initio and classical molecular dynamics of Neon melting at high pressure.
Phys. Rev. B **75**, 214108 (2007).

318. A.Grigoriev and R.Ahuja
Molecular Electronics Devices (Book Chapter)
Nano and Molecular Electronics Handbook
editor S.E. Lyshevski, CRC Press, 2007.
ISBN : 9780849385285



319. S.Arapan, J.Almeida and R.Ahuja
Formation of sp^3 hybridized Bonds and stability of $CaCO_3$ at Very High Pressure
Phys. Rev. Lett. **98**, 268501 (2007).

320. C.Moyses Arujo, R.H. Scheicher, P.Jena and R.Ahuja,
On the structural and energetic properties of the hydrogen absorber : $Li_2Mg(NH)_2$
Appl. Phys. Lett. **91**, 091924 (2007).

321. L.Koci, L.Vitos and R.Ahuja
Ab initio calculations of the elastic properties of ferropericlase $Mg_{(1-x)}Fe_xO$ ($x<0.25$)
Physics of the Earth and Planetary Interiors **164**, 177 (2007).

322. Z.Sun, S.Krysta, D.Music, R.Ahuja and J.M.Schnider
Structure of the Ge-Sb-Te phase-change materials studied by theory and experiment
Solid State Commun. **143,** 240 (2007).

323. A.L.Rosa and R.Ahuja
Tuning the ferromagnetism in Mn-Zn-O by intrinsic defects
J. Phys.: Condens. Matter **19,** 386232 (2007).

324. A.L.Rosa and R.Ahuja
Ferromagetism in Cu-doped GaN
Appl. Phys. Lett. **91**, 232109 (2007).

325.Wei Luo, Rajeev Ahuja, Yang Ding, and Ho-kwang Mao,
Unusual lattice dynamics of vanadium under high pressure,
PNAS (the Proceedings of the National Academy of Sciences,USA), **104**, 16428 (2007).

326.(a) Andreas Blomqvist , C Araujo , Pornjuk Srepusharawoot , Rajeev Ahuja,
Li-decorated metal-organic framework-5, a route to achieve a suitable hydrogen storage medium,
PNAS (the Proceedings of the National Academy of Sciences,USA), **104**, 20173 (2007).

326(b) above paper was selected as one of the highlight paper for that issue.

327.L. Dubrovinsky, N. Dubrovinskaia, W.A.Crichton, A.S. Mikhaylushkin, S.I.Simak, I.A.Abrikosov, J. S. de Almeida, R.Ahuja, W.Luo and B.Johansson
Noblest of all metals is structurally unstable at high pressure
Phys. Rev. Lett. **98**, 045503 (2007).

328. E.I.Isaev, S.I.Simak, I.A.Abrikosov, R.Ahuja, A.I.Lichtenstein, Y.K.Vekilov and B.Johansson
Phonon related properties of transition metals, their carbides, and nitrides: A first-principles study
J. Appl. Phys. **101,** 123519 (2007).

329. K. Kádas, L. Vitos, R. Ahuja, B. Johansson, J. Kollár,
Temperature dependent elastic properties of alpha-beryllium from first principles,
Phys. Rev. B **76,** 235109 (2007)

330.C.M. Araujo , A. Blomqvist and R. Ahuja,
Ti-induced destabilization of $NaBH_4$ from first-principles theory
J. Phys.: Condens. Matter. **20,** 122202 (2008).

331. S.Gowtham, R.H Scheicher, R.Pandey, S.P.Karna and R.Ahuja
First-principles study of physisorption of nucleic acid bases on small-diameter carbon nanotubes
Nanotechnology **19,** 125701 (2008).

332. L.Koci, A.B.Belonoshko and R.Ahuja
Ab initio and classical molecular dynamics calculations of the high pressure Melting of Ne
J.Phys. : Condens. Matter 12, 012005 (2008).

333. D.Y.Kim, S.Kwon and R.Ahuja,
Ab initio study of the pressure effects on $R_2Mo_2O_7$
*J. Phys. and Chem. of Solids **69,** 2245 (2008)*

334. H. He, R.H Scheicher, R.Pandey, A.R.Rocha, S. Sanvito, A.Greigoriev R.Ahuja and S.P.Karna
Functionalized nanopore-embedded electrodes for rapid DNA sequencing
J. Physical Chem. **C 112**, 3456 (2008).

335. Nishad A. Phatak, Shrinivas R. Kulkarni, Vadym Drozd, Surendra K. Saxena, Liwei Deng, Yingwei Fei, Jingzhu Hu, Wei Luo and Rajeev Ahuja,
Synthesis and compressive behavior of Cr_2GeC up to 48 GPa,
*J. Alloys and Compounds **463,** 220 (2008).*

336. C.M.Fang and Rajeev Ahuja
Local structure and electronic-spin transition of Fe-bearing $MgSiO_3$ perovskite up to

the earth's lower mantle conditions,
Physics of the Earth and Planetary Interiors **166,** 77 (2008).

337. C.Moyses Arujo, R.H. Scheicher and R.Ahuja,
Thermodynamic analysis of hydrogen sorption recactions in Li-Mg-N-H systems
***Appl. Phys. Lett*. 92**, 021907 (2008).

338. K. Kádas, L. Vitos and R. Ahuja
Theoretical evidence of a superconducting transition in doped silicon and germanium driven by a variation of chemical composition
Appl. Phys. Lett*. *92, 052505(2008).

339. N.Souza Dantas, J. S. de Almeida, R.Ahuja, C.Persson and A.Ferreira da Silva,
Novel semiconducting materials for optoelectronic applications: $Al_{1-x}Tl_xN$ alloys
Appl. Phys. Lett*. *92, 121914 (2008).

340.(a) F.Ding, P.Larsson, A.Larsson, R.Ahuja, H.Duan, A.Rosen and K.Bolton
The Importance of Strong Carbon-Metal Adhesion for Catalytic Nucleation of
Single-Walled Carbon Nanotubes
Nano Letters 8, 463 (2008).

340. (b) Above paper is selected as **RESEARCH HIGHLIGHTS in NATURE Nanotechnology**.
Title of the highlight was **Nanotubes: Growth control**
Nature Nanotechnology (2008). doi:10.1038/nnano.2008.21

341. L. Koči, R. Ahuja, L. Vitos, and U. Pinsook
Melting of Na at high pressure from ab initio calculations
Phys. Rev. B **77**, 132101 (2008).

342. S.R.Kulkarni, R. S. Vennila, N.A.Phatak, S.K.Saxena, C.S.Zha, T. El-Raghy,
M.W.Barsoum, W.Luo and R.Ahuja,
Study of Ti_2SC under compression up to 47 GPa
J. Alloys and Compounds ***448,*** *L1 (2008).*

343. D.Y. Kim, S. Lebègue, C. Moysés Araújo, B. Arnaud, M. Alouani, and R. Ahuja
Structurally induced insulater-metal transition in solid oxygen : A quasiparticle investigation
Phys. Rev. B **77**, 092104 (2008).

344.P. Larsson, C.Moyses Araujo, J.A.Larsson, P.Jena and R.Ahuja,
Role of Catalysts in Dehydrogenation of MgH_2 Nanoclusters,
PNAS (the Proceedings of the National Academy of Sciences,USA) **105,** 8227 (2008).

345. K. Kádas, L.Vitos and R. Ahuja,
Elastic properties of iron-rich hcp Fe-Mg alloys up to Earth's core pressures
Earth and Planetary Science Letters 271, *221 (2008).*

346.U.Pinsook, R.Scheicher, R.Ahuja and S. Hannongbua,
Internal vibrations of Li(NH3)4+ complex analyzed from ab initio,
density functional theory, and classical spring network model
J. Phys. Chem. A 112, *5323 (2008).*

347.Z.Sun, J.Zhou, A.Blomqvist and R.Ahuja,
Local Structure of Liquid $GeSb_2Te_4$ for rewriteable data storage
J.Phys. : Condens. Matter **20,** 205102 (2008).

348. R.H. Scheicher, D.Y.Kim, S. Lebègue, B. Arnaud, M. Alouani and R.Ahuja
Cubic Metallic Phase of Aluminum Hydride Showing Improved Hydrogen Desorption
Appl. Phys. Lett. **92,** 201903 (2008).

349. A.Modin, K.Kvashnina, S.M.Butorin, L.Werme, J.Nordgren, S.Arapan, R.Ahuja,
A.Fallberg and M.Ottosson,
Electronic structure of Cu_3N films studied by soft x-ray spectroscopy
J.Phys. : Condens. Matter **20,** 235212 (2008).

350.A.Phusittrakool, T.Bovornratanaraks, R.Ahuja and U.Pinsook,
High Pressure structural phase transition in Sr from ab initio calculations,
Phys. Rev. B. *77, 174118 (2008).*

351. W.Luo, C.M.Fang and R.Ahuja,
Nanolayered MAX Phases from ab initio calculations,
Int. J. Mod. Phys. B 22, 4495 (2008).

352.M.Magnuson, O.Wilelmsson, M.Mattesini, S Li, R.Ahuja, O.Eriksson,
H. Högberg, L.Hultman, and U.Jansson,
Anisotrpy in the electronic structure of V_2GeC investigated by Soft x-ray
emission spectroscopy and first principles theory,
Phys. Rev. B*.78, 035117 (2008).*

353. L. Koci, Y. Ma, A.R. Oganov, P. Souvatzis and R. Ahuja,
Elasticity of the superconducting metals V, Nb, Ta, Mo, and W at high pressure
Phys. Rev. B. 77, 214101 (2008).

354. J. Holmes, Z. Li, J. Larsson, R. Ahuja, P. Larsson, T. Joseph, J. O'Byrne, M. Morris,
& G. Attard,
Cu/Mo Nanocomposite Particles as Catalysts for the Growth of Bamboo-Structured Carbon
Nanotubes
J. Phys. Chem. C. 112, *12201 (2008).*

355. L. Koci, A.B.Belonoshko and R. Ahuja,
The impact of system restriction in molecular dynamics applied to melting of Ne at high
Pressure,
Comp. Mat. Sci. **44,** 605 (2008).

356. L. Koci, D.Y.Kim, J.Almeida, M.Mattesini, E.Isaev and R. Ahuja
Mechanical stability of TiO_2 polymorphs under pressure : ab initio calculations
J.Phys. : Condens. Matter**. **20, 345218 (2008).

357.M. D. Deshpande, R. H. Scheicher, R. Ahuja and R. Pandey
Binding strength of sodium ions in cellulose for different water contents
J. Phys.Chem. B.112, 8985 (2008).

358.Z.Sun, J.Zhou, A.Blomqvist, B.Johanson and R.Ahuja,
Fast crysallization of chalcogenide glass for rewritable memories
***Appl. Phys. Lett.* 93,** 061913 (2008).

359. D.Y.Kim, R. H. Scheicher, S. Lebègue, J. Prasongkit, B. Arnaud, M. Alouani, and R. Ahuja
Crystal structure of the pressure-induced metallic phase of SiH_4 *ab initio* theory
PNAS (the Proceedings of the National Academy of Sciences,USA) **105,** 16454 (2008).

360. D.Y. Kim, R. H. Scheicher and R. Ahuja
Dynamical stability of the cubic metallic phase of AlH_3 at ambient pressure: Density functional calculations
***Phys. Rev. B* 78**, 100102(R) (2008).

361.P. Srepusharawoot, C. M. Araujo, A. Blomvist, R. H. Scheicher, and R. Ahuja
A comparative investigation of H2 adsorption strength in Cd- and Zn-based Metal Organic Framework-5
***Journal of Chemical Physics* 129,** 164104 (2008).

362. Z.Sun, J.Zhou, HJ Shin, A.Blomqvist and R.Ahuja,
Stable nitride complex and molecular nitrogen in N doped amorphous Ge2Sb2Te5
***Appl. Phys. Lett.* 93,** 241908 (2008).

363. J.Zhou, Z.Sun, L.H. Xu and R.Ahuja,
Effect of dopants on the structure and properties of Ge2Sb2Te5 studied by Ab initio calculations
Solid State Commun. **148,** 113 (2008).

364. S.Arapan, H.K.Mao and R.Ahuja,
Prediction of incommensurate crystal structure in Ca at high pressure
PNAS (the Proceedings of the National Academy of Sciences,USA) **105,** 20627 (2008).

365.X.Peng and R.Ahuja
Symmetry Breaking Induced Bandgap in Epitaxial Graphene Layers on SiC
Nano Letters 8, 4464 (2008).

366.M.Mattesini, E.Buforn, A.Udias, L.Vitos and R.Ahuja,
An ab initio study of S-substituted iron-nickel-silicon alloy at the Earth's inner core pressure
High Press. Res. **28,** 437 (2008).

367.H.Shi, W.Luo, B.Johansson and R.Ahuja,
First-principles calculations of the electronic structure and pressure-induced magnetic transition in siderite FeCO3
***Phys. Rev. B* 78,** 155119 (2008).

368. Z.Nabi and R.Ahuja,
Ferromagnetism in (Mn,Li) co-doped CdSe
***Euro Phys. Lett.* 84,** 57012 (2008).

369. R.springell, B.Detlefs, G.H.Lander, R.C.C.Ward, R.A.Cowley, N.Ling, W.Goetze, R.Ahuja, W.Luo and B.Johansson,
Elemental engineering : Epitaxial uranium thin films
***Phys. Rev. B* 78,** 193403 (2008).

370.W.Luo and R. Ahuja
Structural Phase Transition in Zircon ($ZrSiO_4$)
***J.Phys. : Condens. Matter,* 121,** *0220014 (2008).*

371. W.Luo, J.Almeida, J.M.O.Guillen and R.Ahuja
Electronic Structure of a Thermoelectric Material : $CsBi_4Te_6$
J. Phys. Chem. Solids ***69,*** *2274 (2008).*

372.S.Li, R.Ahuja, M.W.Barsoum, P.Jena & B.Johansson,
Optical Properties of Ti_3SiC_2 and Ti_4AlN_3
***Appl. Phys. Lett.* 92,** 221907 (2008).

373.B.L. Ahuja, G. Arora, G. Ahmed, A. Rathor, V. Sharma, K. Kádas and R. Ahuja,
A study of electron momentum density and charge transfer in W-Cu system,
***J. Alloys and Compounds* 467,** 595 (2009).

374. S.Arapan, N.V. Skorodumova and R.Ahuja,
Determination of the structural parameters of an incommensurate phase from first principles: The case of Sc-II
***Phys. Rev. Lett.* 102,** 085701 (2009).

375.Z.Sun, J.Zhou, A.Blomqvist, B.Johanson and R.Ahuja,
Formation of large voids in amorphous phase-change memory $Ge_2Sb_2Te_5$ alloy
***Phys. Rev. Lett.* 102,** 075504 (2009).

376 (a). Q.Zeng, Y.Ding, W.L.mao W.Luo, A.Blomqvist, R.Ahuja, W.Yang J.Shu, S.V. Sinogeikin,Y.Meng, D.L.Brewe, J.Z.Jiang and H.K.Mao,
Novel substitutional alloy of Ce and Al
PNAS (the Proceedings of the National Academy of Sciences,USA) **106,** 2515 (2009).

376(b). above paper was selected as one of the highlight paper for that issue.

377.Jianhui Wang, Tao Liu, Guotao Wu, Wen Li, Yongfeng Liu, C. Moysés Araújo, Ralph H. Scheicher, Rajeev Ahuja, Zhitao Xiong, Ping Yang, Mingxia Gao, Hongge Pan and Ping Chen
Potassium Modified $Mg(NH_2)_2$-2LiH System for Hydrogen Storage
***Angew Chem Intl Ed*. 48,** 5828 (2009).

378. A.Zaoui, M.Ferhat and R.Ahuja,
Magnetic properties of (ZnO)1/(CuO)1 (001) superlattice from first-principles theory
***Appl. Phys. Lett.* 94**, 102102 (2009).

379. Z.Sun, J.Zhou and R.Ahuja
Ab initio study of the phase stability and mechanical properties of 5d transition metal nitrides MN2
***J. Alloys & Comp*. 472,** 425 (2009).

380. L.Koci, A.B.Belonoshko and R.Ahuja,
Ab initio calculations of hcp and bcc Fe at extreme conditions,
***High Temp.-High Press.*38,** 37 (2009).

381. X.Peng and R.Ahuja
Non-transition-metal Doped Diluted Magnetic Semiconductors
***Appl. Phys. Lett.* 94**, 102504 (2009).

382. P. A. Berseth, A.G. Harter, R. Zidan, A. Blomqvist, C.M. Araújo, R.H. Scheicher, R.Ahuja and P. Jena
Carbon nanomaterials as catalysts for hydrogen uptake and release in $NaAlH_4$
***Nano Letters* 9**, 1501 (2009).

383.M. Mattesini, R.Ahuja, S.Li, H.W.Hugosson, B.Johansson and O.Eriksson
Electronic structure and optical properties of C_{60}
***Physica B* 404,** 1776 (2009).

384. J. Nisar, R. H. Scheicher, X. Peng and R. Ahuja,
Stability of ferromagnetic phase in Fe-doped AlH_3
***Euro Phys. Lett.* 85,** 67006 (2009).

385. A.Zaoui, M.Ferhat and R.Ahuja,
Magnetism and band gap narrowing in Cu-doped ZnO
***Appl. Phys. Lett.* 94,** 142503 (2009)

386. P.Srepusharawoot, R.Scheicher, C.M. Araujo, A.Blomqvist, U. Pinsook, R. Ahuja,
Ab initio study of hydrogen adsorption in Covalent Organic Framework -1
***J. Phys. Chem. C.* 113,** 8498 (2009).

387. M.Ramzan and R.Ahuja
Ab initio molecular dynamics study of the hydrogen-deuterium exchange in bulk lithiumborohydride (LiBH4)

Appl. Phys. Lett.**94,** 141903 (2009).

388. M. Ramzan, F. Silvearv, A. Blomqvist, R.H. Scheicher, S.Lebegue and R.Ahuja
Structural and energetic analysis of the hydrogen storage materials LiNH2BH3 and NaNH2BH3 from ab initio calculations
Phys. Rev. B. **79,** 132102 (2009).

389. K.Benyahia, Z.Nabi, R.Ahuja and A. Khalfi
Magneto-optical Kerr effect (MOKE) of the rare-earth silicide ErSi2 using ab-initio calculations
Current Applied Physics 9, 925 (2009).

390. M.Ramzan S.Lebegue and R.Ahuja
Ab initio study of lithium and sodium iron fluorophosphate cathodes for rechargeable batteries
Appl. Phys. Lett. **94,** 151904 (2009).

391. C.M. Araujo, A.Blomqvist, R.H. Scheicher, P.Chen and R.Ahuja
Superionicity in the hydrogen storage material Li2NH: Molecular dynamics simulations
Phys. Rev. B.**79,** 172101 (2009).

392. M.Ramzan T.Hussain and R.Ahuja
Hydrogen diffusion in bulk and nanoclusters of MgH2 and the role of catalysts on the basis of ab initio molecular dynamics
Appl. Phys. Lett.**94,** 221910 (2009).

393. J.Almeida, D.Y.Kim, C.Ortiz, M. Klintenberg and R.Ahuja
On the dynamical stability and metallic behavior of YH3 under pressure
Appl. Phys. Lett.**94,** 251913 (2009).

394. D.Y.Kim, R.H.Scheicher and R.Ahuja
Predicted High-Temperature Superconducting State in the Hydrogen-Dense Transition-Metal Hydride YH_3 at 40 K and 17.7 GPa
Phys. Rev. Lett. **103,** 077002 (2009).

395. K.Kadas, L.Vitos, B.Johansson & R.Ahuja
Stability of body-centered cubic iron-magnesium alloys in the Earth's inner core
PNAS (the Proceedings of the National Academy of Sciences,USA) **106,** 15560 (2009).

396. L.Huang, C.M. Araujo and R.Ahuja
Magnetic and electronic properties of 3d transition-metal-doped In2O3: An ab initio study
Euro Phys. Lett.**87,** 27013 (2009).

397. M.Ramzan and R.Ahuja
Ferromagnetism in the potential cathode material LiNaFePO4F
Euro Phys. Lett.**87,** 18001 (2009).

398. M.Ramzan and R.Ahuja

Ab initio molecular dynamics study of the hydrogen diffusion in sodium and lithium hydrides
J. Appl. Phys.**106,** 016104 (2009).

399. J.Schiessling, A.Grigoriev, R.Fasel, R.Ahuja and P.A.Bruhwiler
Interplay of covalent bonding and correlation effects at molecule-metal contacts
Chem. Phys. Lett. 478, 191 (2009).

400. M.Ramzan, S.Lebegue, P.Larsson and R.Ahuja
Structural, magnetic and energetic properties of Na2FePO4F, Li2FePO4F, NaFePO4F and LiFePO4F from ab initio calculations
J. Appl. Phys.**106,** 043510 (2009).

401. C.Århammar, C.M.Araujo and R.Ahuja
Energetics of Al doping & intrinsic defects in monoclinic and cubic zirconia :
Frirst principles calculations
Phys. Rev. B 80, 115208 (2009).

402. H.Shi, W.Luo, B.Johansson and R.Ahuja
Electronic and elastic properties of CaF2 under high pressure from ab initio calculations
J.Phys. : Condens. Matter 21, 415501 (2009).

403. C.J. Glover, T. Schmitt, M. Mattesini, M. Adell, L. Ilver, J. Kanski, L. Kjeldgaard, M. Agåker, N. Mårtensson, R. Ahuja, J. Nordgren, J.-E. Rubensson
Stationary and dispersive features in resonant inelastic soft X-ray scattering at the Ge 3p resonances
J. Elect. Spect. Rel. Pheno.**,** ***173,*** 103 (2009).

404. K. Benyahia, Z.Nabi, R.Ahuja,F.Boukabrine and A.Khalfi
Ab-initio calculations of the optical and magnetic properties of erbium silicide ErSi2
J.Phys. Chem. Sol. **70,** 1378 (2009).

405. M.Ramzan and R.Ahuja
High pressure and temperature study of hydrogen storage material BH3NH3 from ab initio calculations
J. Phys. Chem. Solids **71,** 1137 (2010).

406. L. Huang, M. Ramzan, L. Vitos, B. Johansson, and R. Ahuja
Anomalous temperature dependence of elastic constant c44 in V, Nb, Ta, Pd, and Pt
J. Phys. Chem. Solids **71,** 1065 (2010).

407. A.Blomqvist, C.M. Araujo, R.H. Scheicher, L. Wein, P.Chen and R.Ahuja
Hydrogen as promoter and inhibitor of superionicity: A case study on Li-N-H systems
*Phys. Rev. B.***82,** 024304 (2010).

408. D.Y.Kim and R.Ahuja
Ab initio study on pressure-induced change of effective Coulomb interaction in superconducting yttrium

***Appl. Phys. Lett.* 96,** 022510 (2010).

409. O. D. Jayakumar , S. N. Achary , K. G. Girija , A.K.Tyagi, C. Sudakar , G. Lawes , R. Naik , J. Nisar , X. Peng and R. Ahuja
Theoretical and experimental evidence of enhanced ferromagnetism in Ba and Mn co-substituted BiFeO3
***Appl. Phys. Lett.* 96,** 032903 (2010).

410. Z.Sun, J.Zhou, A.Blomqvist, B.Johanson and R.Ahuja,
Comment on Formation of large voids in amorphous phase-change memory alloys, Reply
***Phys. Rev. Lett.* 104,** 019602 (2010).

411. B.Sa, N. Miao, J.Zhou, Z. Sun and R. Ahuja
Ab initio Study of the Structure and Chemical Bonding of Hexagonal Ge3Sb2Te6
***Phys. Chem. Chem. Phys.* 12,** 1585 (2010).

412. B. Sa, N. Miao, J. Zhou, Z. Song, Z. Sun and R. Ahuja
Phase Stability and Electronic Structure of $Si_2Sb_2Te_5$ Phase-Change Material
J. Phys. Chem. Solids **71,** 1165 (2010).

413. S. Li, R. Ahuja, C.M. Araújo, B. Johansson and P. Jena
Dehydrogenation associated with Ti catalyst in sodium alanate
J. Phys. Chem. Solids **71,** 1073 (2010).

414. P.Larsson, R.Ahuja, A.Livat and J.Thomos
Structural and electrochemical aspects of Mn-substitution into
Li2FeSiO4 from DFT calculations
*Comp. Mat. Sci.***47,** 678 (2010).

415. L.Huang, F.Silvreav, C.M.Araujo and R.Ahuja
Defect induced strong ferromagnetism in Cr doped In2O3 from first principles theory
Sol. Stat. Commun. **150,** 663 (2010).

416. D.Y.Kim, R. H. Scheicher, H.K.Mao, T.W.Kang and R. Ahuja
General trend for pressurized superconducting hydrogen-dense materials
PNAS (the Proceedings of the National Academy of Sciences,USA) **107,** 2793 (2010).

417. J.Nisar, X.Peng and R.Ahuja
Origin of ferromagnetism in molybdenum dioxide from ab initio calculations
Phys. Rev. B 81, 012402 (2010).

418. J.Nisar, C.M.Araujo and R.Ahuja

Structural, electronic and energetic properties of water adsorbed on ☙-Si3N4 (0001) Surface:

First-principles calculations
Surf. Sci. **604**, 616 (2010).

419. L. Qiu , J. Zhou, X. Cheng and R.Ahuja
Electrochemical deposition of Bi_2Te_3-based thin films
J. Phys. Chem. Solids **71,** 1131 (2010).

420. J. Prasongkit, A. Grigoriev, G. Wendin and R.Ahuja
Cumulene molecular wire conductance from first principles
*Phys. Rev. B.***81,** 115404 (2010).

421. Z.M.Sun, R.Ahuja and J.E.Lowther
Mechanical properties of Vanadium Carbide and a ternary Vanadium Tungsten Carbide
Sol. Stat. Commun. **150,** 697 (2010).

422. L.Huang, C.Århammar, C.M.Araujo, F.Silvreav and R.Ahuja
Tuning magnetic properties of In2O3 by control of intrinsic defects
Euro Phys. Lett. **89,** 47005 (2010)

423. Z.Sun, J.Zhou, A.Blomqvist, B.Johanson and R.Ahuja,
Comment on Formation of large voids in amorphous phase-change memory alloys, Reply
Phys. Rev. Lett. **104,** 019604 (2010).

424. J. Holmes, J. O'Byrne, T. Joseph, J. Larsson, P. Larsson, R. Ahuja and Z. Li
Growth of Carbon Nanotubes from Heterometallic Palladium and Copper Catalysts
Journal of Physical Chemistry C **114,** 8115 (2010).

425**.** C. Moysés Araújo and R. Ahuja,
Electronic Structure and High-Pressure Behavior of Solids in *Thermodynamics Properties of Solids: Experiment and Modeling,* eds. S. L. Chaplot, R. Mittal, and N. Choudhury (WILEY-VCH, Weinheim), page:269 (2010).

426. M. Mattesini, A. B. Belonoshko, E. Buforn, M. Ramírez, S. I. Simak, A. Udías, H.K.Mao and R. Ahuja
Hemispherical Anisotropic Patterns of the Earth's Inner Core
PNAS (the Proceedings of the National Academy of Sciences, USA) ***107,*** *9507 (2010)*.

427. B.Sa, N. Miao, J.Zhou, Z. Sun and R. Ahuja
Investigation on $Ge_{5-x}Sb_xTe_5$ phase-change materials by first-principles method
Applied Physics A **99,** 961 (2010).

428. O. D. Jayakumar, S. N. Achary, C. Sudakar, R. Naik, H. G. Salunke, Rekha Rao, X. Peng, R. Ahuja and A. K. Tyagi
Experimental and theoretical investigations on magnetic behavior of (Al,Co) co-doped ZnO nanoparticles
Nanoscale **2,** 1505 (2010).

429. J.Nisar and R.Ahuja

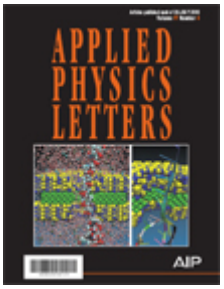
Structure behavior and equation of state (EOS) of Ni_2P and $(Fe_{1-x}Ni_x)_2P$ (allabogdanite) from First-principles calculations
Earth and Planetary Science Letters **295,** 578 (2010).

430. Wendy Mao , Lin Wang , Yang Ding , Wenge Yang , Wenjun Liu , Duck Young kim , Wei Luo , Rajeev Ahuja , Yue Meng , Stanislav Sinogeikin , Jinfu Shu & Ho-Kwang Mao,
Distortions and Stabilization of Simple Cubic Calcium at High Pressure and Low Temperature
PNAS (the Proceedings of the National Academy of Sciences, USA) ***107,*** *9965 (2010)*.

431. B.Sa, N. Miao, J.Zhou, Z. Sun, Z.Song, A.Blomqvist and R. Ahuja
First-principles investigation on the phase stability and chemical bonding of *m*InSb·*n*InTe phase-change random alloys
Sol. Stat. Commun.**150,** 1375 (2010).

432. Wei Luo, Börje Johansson , Olle Eriksson , Sergiu Arapan , Petros Souvatzis , Mikhail Katsnelson & Rajeev Ahuja
Dynamical stability of body centre cubic iron at the Earth's core conditions
PNAS (the Proceedings of the National Academy of Sciences, USA) ***107,*** *9962 (2010)*.

433. Y. He , L. Shao , R. Scheicher, A. Grigoriev , R. Ahuja , S. Long , Z. Ji , Z. Yu , M. Liu
Differential Conductance as a Promising Approach for Rapid DNA Sequencing with Nanopore-embedded Electrodes
Appl. Phys. Lett. **97,** 043701 (2010).



featured as cover image included in August 9, 2010.

434. C. M. Araujo, M. Kapilashrami, X. Jun, O. D. Jayakumar, S. Nagar, Y. Wu, C. Århammar, B.Johansson, L. Belova, R. Ahuja, G. A. Gehring, and K. V. Rao
Room temperature ferromagnetism in pristine MgO thin film
Appl. Phys. Lett. **96,** 232505 (2010).

435. M. Ramzan, S. Lebegue, and R. Ahuja
Electronic structure and metalization of a silane-hydrogen system under high pressure investigated using density functional and GW calculations
Phys. Rev. B.**81,** 233103 (2010).

436. M.Ramzan and R.Ahuja
$M_{N+1}AX_N$ (M = Ti, A = Al, X = H) phase class materials with hydrogen: Ti_4AlH_3 and Ti_3AlH_2
Appl. Phys. Lett. **96,** 261906 (2010).

437. X.Peng and R.Ahuja
The epitaxial graphene monolayer and bilayers on Ru(0001)
***Phys. Rev. B*.82,** 045425 (2010).

438. M.Ramzan, S. Lebegue and R.Ahuja
Crystal and electronic structures of lithium fluorosulphate based materials for lithium-ion batteries
***Phys. Rev. B*82,** 125101 (2010).

439. P.Srepusharawoot, A.Blomqvist, C.M. Araujo, R.Scheicher & R. Ahuja,
One-dimensional polymeric carbon structure based on five-membered rings in alkaline earth metal dicarbides BeC_2 and MgC_2
***Phys. Rev. B*82,** 125439 (2010).

440. J.Nisar and R.Ahuja
Equation of state (EOS) and Collapse of magnetism in Iron-rich meteorites at high pressure from ab initio calculations
Physics of the Earth and Planetary Interiors ***182,*** 175 (2010).

441. W. Li, G. Wu, C.M.Araujo, R. H. Scheicher, A. Blomqvist, R. Ahuja, Z. Xiong, Y. Feng and P. Chen

Li^+ ion conductivity and diffusion mechanism in α-Li_3N and β-Li_3N

Energy & Environmental Science **3**, 1524 (2010).

442. C. Århammar, C.M. Araujo, K.V.Rao, B.Johansson and R.Ahuja
Energetics and magnetic properties of V-doped MgO bulk and (001) surface: A GGA, GGA+U, and hybrid density functional study
***Phys. Rev. B*.82,** 134406 (2010).

443. S. M. Jafri, T. Blom, K. Leifer, M. Strömme, H. Löfäs, A. Grigoriev, R. Ahuja and K. Welch
Assessment of a nanoparticle bridge platform for molecular electronics measurements
Nanotechnology **21**, 435204 (2010).

444. M.Ramzan, S. Lebegue and R.Ahuja
Transition metal doped MgH_2: a material to potentially combine fuel-cell and battery technologies
International Journal of Hydrogen Energy **35,** 10373 (2010).

445. W. Li, R. H. Scheicher, C.M. Araujo, G. Wu, A. Blomqvist, C.Wu, R. Ahuja, Y. Feng and P. Chen
Understanding from First Principles why $LiNH_2BH_3{\cdot}NH_3BH_3$ Shows Improved Dehydrogenation over $LiNH_2BH_3$ and NH_3BH_3
***Journal of Physical Chemistry C* 114,** 19089 (2010).

446. A. Grigoriev, M. Stener, L. Kjeldaard, P. Decleva, R. Ahuja,
J. Nordgren, P.A. Bruhwiler, J. Schiessling and T. Balasubramanian,
The Role of Charge-Charge Correlations and Covalent Bonding in the Electronic Structure of Adsorbed C_{60}/ C_{60}/Al
***Journal of Physical Chemistry C* 114,** 18686 (2010).

447. A.Blomqvist, G.K.Palsson, C.M.Araujo, R.Ahuja and B.Hjorvarsson
Significance of self-trapping on hydrogen diffusion
***Phys. Rev. Lett.* 105,** 185901 (2010).

448. S.Arapan and R.Ahuja
High-pressure phase transformations in carbonates
***Phys. Rev.B.*82,** 184115 (2010).

449. Y. He , R. Scheicher, A. Grigoriev , R. Ahuja , S. Long , Z. Huo & M. Liu,
DNA Sequencing with nanopore-embedded bilayer-graphene nanoelectrodes
Solid-State and Integrated Circuit Technology, IEEE, Issue Date: 1-4 Nov. 2010,
page(s): 1483 – 1485, ISBN: 978-1-4244-5797-7.

450. P.Srepusharawoot, A.Blomqvist, C.M. Araujo, R.Scheicher & R. Ahuja
Hydrogen Binding In Alkali-Decorated Iso-Reticular Metal Organic Framework-16 Based On Zn, Mg, And Ca
International Journal of Hydrogen Energy **36,** 555 (2011).

451. K.Kadas, R.Ahuja, B.Johansson, O.Eriksson and L.Vitos
Thermo-physical properties of body-centered cubic iron-magnesium alloys under extreme conditions
Solid State Comun. 151, 203 (2011).

452. (a) R.Ahuja, A.Bolmqvist, P.Larsson, P.Pyykkö and P.Zaleski-Ejgierd
Relativity and the lead-acid battery
***Phys. Rev.Lett.*106,** 018301(2011).

(b) Above paper is selected as **RESEARCH HIGHLIGHTS in NATURE (Nature 469**, 269 (2011) & **The Economist, 398, No. 8716 pp. 75-76 (2011)**

453. M.Ramzan, W.Luo and R.Ahuja
High pressure, Mechanical and Optical properties of ZrW2O8
J. Appl. Phys. 109, 033510 (2011).

454. M.Ramzan, S. Lebegue and R.Ahuja
Hybrid exchange-correlation functional study of the structural, electronic, and mechanical properties of the MAX phases
***Appl. Phys. Lett.* 98,** 021902 (2011).

455. M.Ramzan, S. Lebegue, T.W. Kang and R.Ahuja

Hybrid Density Functional Calculations and Molecular Dynamics Study of Lithium-Fluorosulphate, a Cathode Material for Lithium-Ion Batteries
Journal of Physical Chemistry C.**115,** 2600 (2011).

456. J.Nisar, C.M. Araujo and R.Ahuja
Water Interaction with native defects on rutile TiO2 nanowire: ab-initio calculations
Appl. Phys. Lett. **98,** 083115 (2011)

457. M.Ramzan, S. Lebegue and R.Ahuja,
Correlation effects in the electronic and structural properties of Cr_2AlC
Physica Status Solidi-Rapid Research Letter **5***,* 122 (2011).

458. K.Kadas, H.Zhang, B.Johansson, L.Vitos and R.Ahuja
Thermo-physical properties of iron-magnesium alloys, pp. 69-94 (book Chapter)
Source: Magnesium Alloys - Design, Processing and Properties, Book edited by: Frank Czerwinski, ISBN: 978-953-307-520-4, Publisher: InTech, Publishing date: January 2011.

459. J.Nisar, X.Peng, T.W.Kang and R.Ahuja
Stabilizing the defect-induced dilute magnetic semiconductors: Li-doping in GaN with Ga vacancies
Euro Phys. Lett. **93***,* 57006 (2011).

460. A.Zaoui, A.Belabbes, R.Ahuja & M.Ferhat
Interplay between lattice dynamics and the low pressure phase of simple cubic polonium
*Phys. Lett. A.***375,** 1695 (2011).

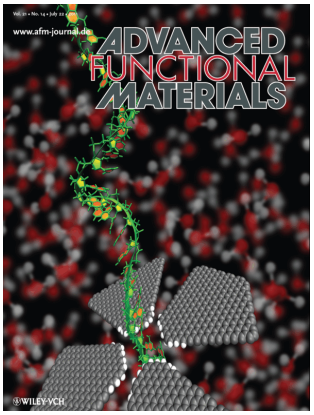
461. Z.Sun, Y.Pan, J.Zhou, B.Sa and R.Ahuja
Origin of p-type conductivity in layered nGeTe: mSb_2Te_3 chalcogenide semiconductors
Phys. Rev.B **83,** 113201 (2011).

462. C. Århammar, A. Pietzsch , N. Bock , E. Holmström , C.M. Araujo , J. Gråsjö , S. Zhao , S. Green , T. Peery , F. Hennies , S. Amerioun , A. Föhlisch , J. Schlappa , T. Schmitt , V. N. Strocov, G. A. Niklasson , D. C. Wallace , J.E. Rubensson , B. Johansson and R. Ahuja
Unveiling the complex electronic structure of amorphous metal oxides
PNAS (the Proceedings of the National Academy of Sciences, USA) **108,** 6355 (2011).

463. J.Nisar, C.Århammar, E.Jämstorp and R.Ahuja
Optical gap and native point defects in kaolinite studied by GGA-PBE, HSE-functional, and GW approach
Phys. Rev. B. **84,** 075120 (2011).

464. M. Krisch , D. Farber , R. Xu , D. Antonangeli , C. Aracne , A. Beraud , T.-C. Chiang , J. Zarestky , D. Y. Kim , E. Isaev , R. Ahuja and B. Johansson
Phonon Spectra for a Anomalous Elemental Metal: Cerium
PNAS (the Proceedings of the National Academy of Sciences, USA) **108,** 9342 (2011).

465. Y. He , L. Shao , R. Scheicher, A. Grigoriev , R. Ahuja , S. Long , Z. Huo & M. Liu
Enhanced DNA sequencing performance through edge-hydrogenation of graphene electrodes
Adv. Funct. Mater. 21, 2674 (2011).



(b) selected as inside front cover image.

466. J. Prasongkit A. Grigoriev, B.Pathak, R. Ahuja and R. Scheicher
Transverse conductance of DNA nucleotides in a graphene nanogap from first principles
Nano Letters **11,** 1941 (2011)

467. B.Pathak, D.Samanta, R.Ahuja and P.Jena
Borane Derivatives: A New Class as Super and Hyperhalogens
ChemPhysChem **12,** 2423 (2011)

468. J. Zhou, Z. Sun, Y. Pan, Z. Song and R. Ahuja
An insight on the intrinsic vacancies in rocksalt structured GeSbTe alloys from ab initio Calculations
Euro Phys. Lett. **95**, 27002 (2011).

469. Z. Sun, J. Zhou, Y. Pan, Z. Song, H.K.Mao and R. Ahuja
Pressure-induced reversible amorphization and an amorphous-amorphous transition in $Ge_2Sb_2Te_5$ phase-change memory material
PNAS (the Proceedings of the National Academy of Sciences, USA) **108,** 10410 (2011).

470. Duck Young Kim, Ralph H. Scheicher, Chris J. Pickard, R.J.Needs and R.Ahuja
Predicted formation of superconducting platinum-hydride crystals under pressure in the presence of molecular hydrogen
Phys. Rev. Lett.**107,** 117002 (2011).
Highlighted in APS Physics, Editor's Suggestion.

471. R.Scheicher, S.Li, C.M. Araujo, A.Blomqvist, R. Ahuja & P.Jena
Theoretical study of C_{60} as catalyst for dehydrogenation in $LiBH_4$
Nanotechnology **22,** 335401 (2011).

472. J.Nisar, B.C.Wang, B.Pathak, T.W.Kang and R.Ahuja

Mo- and N-doped $BiNbO_4$ for photocatalysis Applications
***Appl. Phys. Lett.* 99,** 051909 (2011)

473. C.M.Fang and R.Ahuja
Fe bearing $MgSiO_3$ perovskite uo to the Earth's lower mantle conditions
***Fisica de la Tierra* 23**, 43 (2011).

474. T. Kaewmaraya, Duck Young Kim, S. Leb`egue, Chris J. Pickard, R.J.Needs and R.Ahuja
Theoretical investigation of xenon-hydrogen solids under pressure using ab-initio DFT and GW calculations
***Phys. Rev. B.* 84,** 092101 (2011).

475. H.Löfås, A.Grigoriev, J.Isberg and R.Ahuja
Effective masses and electronic structure of dimond including electron correlation effects in first principles calculations using the GW approximation
AIP *Advances* 1, 032139 (2011).

476. B.Sa, J. Zhou, Z. Song, Z.Sun and R. Ahuja
Pressure induced topological insulating behaviour in the ternary chalcogenide $Ge_2Sb_2Te_5$
***Phys. Rev. B.*84,** 085130 (2011).

477. N.Miao, B.Sa, J. Zhou, Z.Sun and R. Ahuja
Mechanical properties and electronic structure of the incompressible rhenium carbides and nitrides: A first-principles study
***Solid State Comun.*151,** 1842 (2011).

478. T. Hussain, B. Pathak, T. A. Maark, C. Moyses Araujo, R. H. Scheicher and R. Ahuja
Ab initio study of lithium-doped graphane for hydrogen storage
***Euro Phys. Lett.* 96,** 27013 (2011).

479. M.Ramzan, F.Silvearv S. Lebegue and R.Ahuja,
Electronic Structure from First Principles of LiBH4.NH3, Sr(NH2BH3)2 and Li2Al(BH4)5.6NH3 for Hydrogen Storage Applications
***Journal of Physical Chemistry C* 115,** 20036 (2011).

480. B. Li , Y. Ding , D.Y. Kim , R. Ahuja , G. Zou , H.K. Mao
Rhodium dihydride (RhH2) with high volumetric hydrogen density
***PNAS* 108,** 18618 (2011).

481. A. Blomqvist, C. Arhammar, H. Pedersen, F. Silvearv, S. Norgren and R. Ahuja
Understanding the catalytic effects of H_2S on CVD-growth of α-alumina: Thermodynamic gas-phase simulations and Density Functional Theory
***Surface and Coatings Technology* 206,** 1771 (2011).

482. J. Prasongkit, A. Grigoriev, R.Ahuja and G. Wendin

Interference effects in phtalocyanine controlled by H-H tautomerization: Potential two-terminal unimolecular electronic switch
***Phys. Rev.* B84**, 165437 (2011).

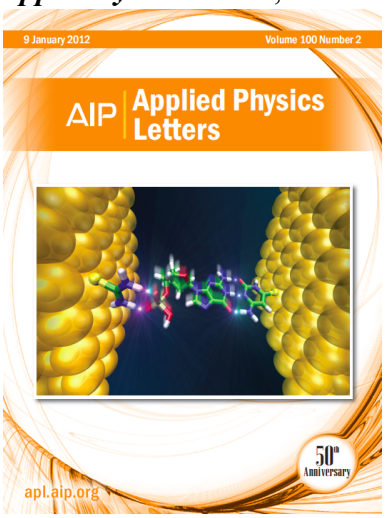
483. Ho-kwang Mao, Yang Ding, Yuming Xiao, Paul Chow, Jinfu Shu, Sébastien Lebègue, Amy Lazickif and Rajeev Ahuja
Electronic dynamics and plasmons of sodium under compression
***PNAS (the Proceedings of the National Academy of Sciences, USA)* 108,** 20434 (2011).

484. M.Ramzan and R.Ahuja,
Role of correlation effects in the superconducting material: InV6S8
***Appl. Phys. Lett*.99**, 221904 (2011).

485. K. Benyahia, Z. Nabi, R. Ahuja and A. Khalfi
Rare-Earth Silicide ErSi2 from First Principles Calculations: Optical, Magnetic and Magheto-Optical Properties, pp. 189-204 (book Chapter)
Source: **Erbium: Compounds, Production and Applications,** Book edited by: Emily K. Byrne
Publisher: Nova Science Publishers, 2011.

486. K.Kadas, R.Ahuja, B.Johansson, O.Eriksson & L.Vitos
Theoretical prediction of the elastic properties of body-centered cubic Fe-Ni-Mg alloys under extreme conditions
Philosophical Magazine 92, 888 (2012).

487. B.Pathak, H.Löfås, J. Prasongkit, A.Grigoriev, R.Ahuja and R. H. Scheicher,
Double-functionalized nanopore-embedded gold electrodes for rapid DNA sequencing
***Appl. Phys. Lett*. 100**, 023701 (2012).



(b) ***Cover Picture of the issue.***

488. B.Pathak, K. Pardhan, T.Hussain, R.Ahuja and P.Jena
Functionalized Boranes for Hydrogen Storage
***ChemPhysChem* 13,** 301 (2012).

489. J.Nisar, B.C.Wang, C.M.Araujo, A. F. Da Silva, T.W.Kang and R.Ahuja
Band gap engineering by anion doping in the Photocatalyst BiTaO4: First principle calculations
International Journal of Hydrogen Energy 37, 3014 (2012).

490. T. Kaewmaraya, B. Pathak, C. M. Araujo, A. L. Rosa and R. Ahuja
Water adsorption on ZnO(10-10): The role of intrinsic defects
***Euro Phys. Lett.* 97,** 17014 (2012)**.**

491. B. Sa, J. Zhou, Z. Sun and R. Ahuja
Strain-induced topological insulating behavior in ternary chalcogenide Ge(2)Sb(2)Te(5)
***Euro Phys. Lett.* 97,** 27003 (2012)**.**

492. H.Zhang, B.Johansson, R.Ahuja and L.Vitos
First principle study of solid solution hardening in steel alloys
***Computational Materials Science* 55**, 269 (2012).

493. J. Zhou, Z. Sun, Y. Pan, Z. Song and R. Ahuja
Ab initio study of antisite defective layered Ge2Sb2Te5
***Materials Chemistry & Physics* 133**, 159 (2012).

494. J.Nisar, B.Pathak, B.C.Wang, T.W.Kang and R.Ahuja
Hole mediated coupling in Sr2Nb2O7 for visible photocatalysis
***Phys. Chem. Chem. Phys.* 14**, 4891 (2012)

495. W. Li, L. Miao, R. Scheicher, Z.Xiong, G.Wu, C. Araujo, A.Blomqvist, R.Ahuja, Y. Feng, P.Chen
Li-Na Ternary Amidoborane for Hydrogen Storage: Experimental and First-Principles Study
***Dalton Transactions.*41,** 4754 (2012).

(b) Cover Picture of the issue.

496.F.Silvreav, A.L.Rosa, S. Lebegue and R.Ahuja
An ab-initio study of (Mn,Al) doped ZnO including strong correlation effects
Physica E **44,** 1095 (2012).

497. Z. Sun, J. Zhou, H.K.Mao and R. Ahuja

Peierls distortion mediated reversible phase transition in GeTe
PNAS (the Proceedings of the National Academy of Sciences, USA) **109,** 5949 (2012).

498. J.Nisar, B.C.Wang, A.F. Da Silva and R.Ahuja
Study of electronic and optical properties of BiTaO4 for photocatalysis
Physica Status Solidi C9, 1593 (2012)**.**

499. T. A. Maark, T. Hussain and R. Ahuja

Structural, electronic and thermodynamic properties of Al and Si doped alpha, beta & gamma

MgH2: density functional & hybrid density functional calculations

International Journal of Hydrogen Energy **37,** 9112 (2012).

500. P.Srepusharawoot, W.Luo, T. Bovornratanaraks, R. Ahuja & U.Pinsook
Evidence of a medium-range ordered phase and Mechanical instabilities in Strontium
Solid State Comunn. **152,** 1172 (2012).

501. Q.Zhao, M.S.Hudson, H.Raghubanshi, R.Scheiher, B.Pathak, C.M.Araujo, A.Blomqvist, B.Johansson & R.Ahuja
Excellent Catalytic Effects of Graphene Nanofibers on Hydrogen Release of Sodium Alanate
The Journal of Physical Chemistry **116,** 10861 (2012).

502. M.Ramzan, S. Lebègue and R.Ahuja,
Electronic and mechanical properties of Cr2GeC with hybrid functional and correlation effects
Solid State Comunn. **152,** 1147 (2012).

503. S. Lebègue, C. Moysés Araújo, D. Y. Kim, M. Ramzan, H.-k. Mao, and R. Ahuja
Semi-metallic dense hydrogen above 260 GPa
PNAS (the Proceedings of the National Academy of Sciences, USA) **109,** 9766 (2012).

504. B.C.Wang, J.Nisar, B.Pathak, T.W.Kang and R.Ahuja
Band Gap Engineering in BiNbO4 for Visible-Light Photocatalysis
Appl. Phys. Lett. **100,** 182102 (2012).

505. J.Nisar, B.Pathak and R.Ahuja
Screened hybrid density functional study on Sr2Nb2O7 for Visible light Photocatalysis
Appl. Phys. Lett. **100,** 181903 (2012).

506. Q.Zhao, B.Pathak and R.Ahuja
Oxygen- and nitrogen-chemisorbed carbon nanostructures for Z-scheme photocatalysis applications
Journal of Nanoparticle Research **14,** 895 (2012).

507. H.B. Lou, Y.K. Fang, Q.S. Zeng, Y.H. Lu, X.D. Wang, Q.P. Cao, K. Yang, X.H. Yu, L. Zheng, Y.D. Zhao, W.S. Chu, T.D. Hu, Z.Y. Wu, R. Ahuja and J.Z. Jiang
Pressure-induced amorphous-to-amorphous configuration change in Ca-Al metallic glasses
Nature-Scientific Reports **2,** 376 (2012).

508.T. Hussain, B. Pathak, M. Ramzan, T. A Maark, and R. Ahuja
Calcium doped graphane as a hydrogen storage material
Appl. Phys. Lett. **100,** 183902 (2012).

509. P.Liu, J.Nisar, B.Pathak and R.Ahuja
Hybrid Density Functional Study on SrTiO3 for Visible Light Photocatalysis
International Journal of Hydrogen Energy **37,** 11611 (2012).

510. W.Sun, W.Luo and R.Ahuja
Role of correlation and relativistic effects in MAX phases
Journal of Materials Science **47,** 7615 (2012)**.**

511. T.Hussain, A.Sarkar and R. Ahuja
Strain induced lithium functionalized graphane as a high capacity hydrogen storage material
Appl. Phys. Lett. **101**, 103907 (2012).

512. D.Y.Kim, P. Srepusharawoot, C. J. Pickard, R. J. Needs, T. Bovornratanaraks, R. Ahuja and U. Pinsook
Phase stability and superconductivity of strontium under pressure
Appl. Phys. Lett. 101, 052604 (2012).

513. R.Scheiher A.Grigoriev and R.Ahuja
DNA sequencing with nanopores from an ab initio perspective
Journal of Materials Science **47,** 7439 (2012)**.**

514. T. Hussain, B. Pathak, T. A Maark, M.Ramzan and R. Ahuja
Functionalization of graphane with alkali and alkaline-earth metals: An insulator to metallic transition
Euro Phys. Lett. **99,** 47004 (2012).

515. M.Dixit, T. A Maark, K. Ghatak, R. Ahuja and S.Pal
Scandium Decorated MOF-5 as Potential Candidate for Room Temperature Hydrogen Storage: A Solution for the Clustering Problem in MOFs
The Journal of Physical Chemistry C **116,** 17336 (2012).

516. J.Hwang, C.Park, K. Choi, M-H. Cha, R.Ahuja, D.W.Kim, D.O.Kim, K. Sagong, U.G.Joung H.Jeong and J.Ihm
Hydrogen storage enhancement via transition metal decoration on metal organic frameworks : A first principles study
Nano 7, 1250044 (2012)**.**

517. C. S. Kong, W. Luo, S. Arapan, P. Villars, S. Iwata, R. Ahuja and K. Rajan
Information-Theoretic Approach for the Discovery of Design Rules for Crystal Chemistry
J. Chem. Inf. Model.**52**, 1812 (2012).

518. M.Ramzan and R. Ahuja
Hybrid Density Functional and Molecular Dynamics Study of Promising Hydrogen Storage Materials: Double Metal Amidoboranes and Metal Amidoborane Ammoniates
***The Journal of Physical Chemistry C*116,** 17351 (2012).

519. J.Nissar, X.Jiang, B.Pathak, J. Zhou, T.W.Kang & R.Ahuja
Semiconducting Allotrope of Graphene
***NanoTechnology* 23,** 385704 (2012)**.**

520. R. Lizarraga, M. Ramzan, C. M. Araujo, A. Blomqvist, R. Ahuja and E. Holmström
Structural characterization of amorphous $YCrO_3$ from first principles
Euro Phys. Lett. **99,** 57010 (2012).

521. B.Sa, J.Zhou, Z.Sun, J.Tominaga & R.Ahuja
Topological insulating in $GeTe/Sb_2Te_3$ phase-change superlattice
Phys. Rev. Lett. **109**, 096802 (2012).

522. M.Ramzan, T.Hussian & R.Ahuja
High pressure phase determination and electronic properties of lithiumamidoborane
Appl. Phys. Lett. **101**, 111902 (2012).

523. J.D.Baran, W.Kolpdziejczk, P.Larsson, R.Ahuja & A.Larsson
On the stability of single-walled carbon nanotubes and their binding strengths
***Theoretical Chemistry Accounts* 131,** 1270 (2012).

524. B.wang, J.Nissar & R.Ahuja
Molecular simulation for gas adsorption at NiO (100) surface
***ACS Applied Materials & Interfaces* 4,** 5691 (2012).

525. Shuanglin Hu, S.-Y. Li, R. Ahuja, C. G. Granqvist, K. Hermansson,G. A. Niklasson and R. H. Scheicher
Optical properties of Mg-doped VO2: Absorption measurements and hybrid functional Calculations
Appl. Phys. Lett. **101**, 201902 (2012).

526. P.Kanhere, J.Nisar, Y.Tang, B.Pathak, R.Ahuja, J.Zheng & Z. Chen
Electronic Structure, Optical Properties, and Photocatalytic Activities of LaFeO3-NaTaO3 Solid Solution
***The Journal of Physical Chemistry C* 116,** 22767 (2012).

527. Q.Zhao, S.Li, B.Pathak, C.M.Araujo, R.Ahuja & P.Jena
C_{60}-mediated hydrogen desorption in Li-N-H systems
***NanoTechnology* 23,**485406 (2012).

528. T. Hussain, T. A Maark, A.D.Sarkar and R. Ahuja
Polylithiated (OLi2) functionalized graphane as a potential hydrogen storage material

Appl. Phys. Lett. **101**, 243902 (2012).

529. S. Bouhou, I. Essaoudi, A. Ainane, F. Dujardin, R. Ahuja and M. Saber
Magnetic Properties of Diluted Magnetic Nanowire
Journal of Superconductivity and Novel Magnetism 26, 201 (2013).

530. P. Dera, J. Nisar, R. Ahuja, S. Tkachev and V. B. Prakapenka
New type of possible high-pressure polymorphism in NiAs-type minerals of the Earth core
Physics and Chemistry of Minerals 40, 183 (2013).

531. T. Kaewmaraya, M. Ramzan, H. Löfås and R. Ahuja
Electronic and optical properties of phase change memory material : $Ge_2Sb_2Te_5$
Journal of Applied Physics 113, 033510 (2013) **.**

532. S. Yılmaz, J. Nisar, Y. Atasoy, E. McGlynn, R. Ahuja, M. Parlak & E. Bacaksız
Defect-induced room temperature ferromagnetism in B-doped ZnO
Ceramics International 39, 4609 (2013).

533. M.Ramzan, Y.G.Li, R.Chimata & R.Ahuja
Electronic, mechanical and optical properties of Y2O3 with hybrid density functional (HSE06)
Computational Materials Science 71, 19 (2013)**.**

534. X. Jiang, J. Nisar, B. Pathak, J. Zhao and R. Ahuja
Graphene oxide as a chemically tunable 2-D material for visible-light photocatalyst applications
Journal of Catalysis 299, 204 (2013).

535. T. Hussain, A. D. Sarkar, T. A. Maark, W. Sun and R. Ahuja
Strain and doping effects on the energetics of hydrogen desorption from the MgH_2 (001) surface
Euro Phys. Lett. **101,** 27006 (2013).

536. X. Jiang, J. Zhao and R. Ahuja
A novel superhard BN allotrope under cold compression of h-BN
Journal of Physics: Condensed Matter 25, 122204 (2013).

537. S. Bouhou, I. Essaoudi, A. Ainane, M. Saber, R. Ahuja and F. Dujardin,
Phase diagram of diluted transverse Ising Nanowire
J.Mag.Mag.Mat.**336,** 75 (2013).

538. P.Liu, J.Nisar, B. Pathak and R. Ahuja
Layered Perovskite Sr2Ta2O7 for Visible Light Photocatalysis: A First Principles Study
The Journal of Physical Chemistry C **117,** 5043 (2013).

539. H. Löfås, A. Grigoriev, J.Isberg & R.Ahuja
Transport coefficients in diamond from ab-initio calculations
Appl. Phys. Lett. **102,** 092106 (2013).

540. Q.Zhao, B.Pathak & R.Ahuja
Energetic and structural analysis of N2H4BH3 inorganic solid and its modified material for hydrogen storage
***International Journal of Hydrogen Energy* 38,** 6718 (2013).

541. S. Bouhou, A.Zaim, A. Ainane, K. Kerouad & R. Ahuja,
Magnetic properties of a ferromagnetic thin film with four spin interaction: A Monte Carlo simulation study
***J.Mag.Mag.Mat.*339,** 127 (2013).

542. **Y. Benhouria,** I. Essaoudi, A. Ainane, M. Saber, R. Ahuja & F. Dujardin,
Monte Carlo Study of Long-Range Interactions of a Ferroelectric Bilayer with Antiferroelectric Interfacial Coupling
***Journal of Superconductivity and Novel Magnetism* 26,** 3075 (2013).

543. H.Löfås, A. Orthaber, J. Burkhard, A.Rouf, A. Grigoriev, S. Ott, R. Ahuja & H.Ottosson,
A New Class of Molecular Conductance Switches Based on the [1,3]-Silyl Migration from Silanes to Silenes
***The Journal of Physical ChemistryC* 117,** 10909 (2013).

544. J. Prasongkit, A. Grigoriev and R. Ahuja
Mechano-switching devices from carbon wire-carbon nanotube junctions
***Phys. Rev.B.*87,** 155434 (2013).

545. S. H. M. Jafri, H. Löfås, J. Fransson, T. Blom, A. Grigoriev, A. Wallner, R. Ahuja,
H. Ottosson & K. Leifer,
Identification of vibrational signatures form short chains of interlinked molecule-nanoparticle junctions obtained by inelastic electron tunnelling spectroscopy
***NanoScale* 5,** 4657 (2013).

546. P. -A. Glans, T. Learmonth, K. E. Smith, S. Ferro, A. De Battisti, M. Mattesini, R. Ahuja & J. Guo
Electronic structure of boron doped diamond: an x-ray spectroscopic study
***Appl. Phys. Lett*. 102,** 162103 (2013).

547. X. Jiang, C. Århammar , L. Peng, J. Zhao and R. Ahuja
The R3-carbon allotrope: a pathway towards glassy carbon under high pressure
***Nature-Scientific Reports* 3,** 1877 (doi:10.1038/srep01877) (2013).

548. D. Benson, Y. Li, W. Luo, R. Ahuja, G. Svensson and U. Häussermann
Lithium and Calcium Carbides with Polymeric Carbon Structures
***Inorg. Chem.* 52,** 6402 (2013).

549. Y-L.Li, W.Luo, Z.Zeng, H.Q.Lin, H.K.Mao & R.Ahuja
Pressure induced superconductivity in CaC_2
PNAS (the Proceedings of the National Academy of Sciences, USA) **110,** 9289 (2013).

550. Y.Li, Y-L. Li, C.M.Araujo, W.Luo & R.Ahuja
Single-layer MoS_2 as efficient photocatalyst
***Catalysis Science & Technology* 3,** 2214 (2013).

551. J. Ångström, R. Johansson, L. H. Rudec, C.Gundlachd, R. H. Scheicher, R. Ahuja, O. Eriksson, T. R. Jensen & M. Sahlberg
Hydrogen storage properties of the pseudo binary Laves phase $(Sc_{1-x}Zr_x)(Co_{1-y}Ni_y)_2$ system
***International Journal of Hydrogen Energy* 38,** 9772 (2013).

552. X. Jiang, J. Zhao, Y-L. Li, R. Ahuja
Tunable assembly of sp^3 cross-linked three dimensional graphene monoliths
***Adv. Funct. Mater.* 23,** 5846 (2013).

553. B.Sa, Z.M.Sun, T. Kaewmaraya, J.Zhou and R.Ahuja
Structural and vibrational properties of layered data storage material: $Ge_2Sb_2Te_5$
Science of Advanced Materials. 5, 1493 (2013).

554. J. Zhu, J.L.Zhang, P.P.Kong, S.J.Zhang, X.H.Yu, J.L.Zhu, Q.Q Liu, X.Li, R.C.Yu, R. Ahuja, W.G.Yang, G.Y.Shen, H.K.Mao, H.M.Weng, X.Dai, Z.Fang, Y.S.Zhao & C.Q.Jin
Superconductivity in Topological Insulator Sb_2Te_3 Induced by Pressure
***Nature-Scientific Reports* 3,** 2016 (2013).

555. Z. Qian, A. D. Sarkar, T. A. Maark, X. Jiang, M. D. Deshpande, M. Bououdina & R. Ahuja
Pure and Li-doped NiTiH: potential anode materials for Li-ion rechargeable batteries
***Appl. Phys. Lett*. 103,** 033902 (2013).

556. S. Heathman, T. Le Bihan, S. Yagoubi, B. Johansson and R. Ahuja
Structural investigation of californium under pressure
***Phys. Rev.B.* 87,** 214111 (2013).

557. R. B. Araujo, R. H. Scheicher, J. S. de Almeida, A.F. da Silva and R.Ahuja
First-principles investigation of Li ion diffusion in Li_2FeSiO_4
***Solid State Ionics* 247-248,** 8 (2013).

558. Y.Li, A. D. Sarkar, B.Pathak & R.Ahuja
Strain induced stabilization of Al functionalization in grephene oxide nanosheets
***Appl. Phys. Lett*. 102,** 243905 (2013).

559. T. Hussain, A. D. Sarkar, T.W.Kang and R. Ahuja
Hexagonal boron nitride sheet decorated by polylithiated species for efficient and reversible hydrogen storage.
***Science of Advanced Materials* 5,** 1960 (2013).

560. Y.Li, T. Hussain, A. D. Sarkar and R. Ahuja

Hydrogen Storage in Ploylithiated BC_3 monolayer sheet
***Solid State Communication* 170,** 39 (2013).

561. T. Hussain, S.Chakraborty and R. Ahuja
Metal Functionalized Silicene for Efficient Hydrogen Storage
***ChemPhysChem* 14,** 3463 (2013).

562. Y.Li, B.Pathak, J.Nisar, Q.Zhao & R.Ahuja
Metal-decorated graphene oxide for ammonia adsorption
***Euro Phys. Lett.* 103,** 28007 (2013).

563. M. Mattesini, A. B. Belonoshko, H.Tkaicic, E. Buforn¸ A. Udías, and R. Ahuja
Candy Wrapper for the Earth's Inner Core
***Nature-Scientific Reports* 3,** 2096 (2013).

564. A. B. Belonoshko, M.Ramzan, H.K.Mao and R. Ahuja
Atomic Diffusion in Solid Molecular Hydrogen
***Nature-Scientific Reports* 3,** 2340 (2013).

565. T.Kaewmaraya, M.Ramzan, W.Sun, M.Sagynbaeva and R.Ahuja
Atomistic study of promising catalyst and electrode material for memory capacitors: Platinum Oxides
***Computational Materials Science* 79,** 804 (2013).

566. M.Ramzan, T.Kaewmaraya and R.Ahuja
Molecular dynamics study of amorphous Ga-doped In_2O_3: a promising material for phase change memory devices
***Appl. Phys. Lett*. 103,** 072113 (2013).

567. A.Srivastava, N.Tyagi & R.Ahuja
First principle study of structural and electronic properties of gallium based nanowires
***Solid State Sciences* 23,** 35 (2013).

568. J.Nisar, Z.Topalian, A. D. Sarkar, L. Österlund and R. Ahuja
TiO_2 based gas sensor : a possible application to SO_2
***ACS Applied Materials & Interfaces* 5,** 8516 (2013).

569. P.Liu, J.Nisar, B.Sa, B.Pathak & R.Ahuja
Anion-anion mediated coupling in layered pervoskite $La_2Ti_2O_7$ for visible light photocatalysis
***The Journal of Physical ChemistryC* 117,** 13845 (2013).

570. J. Prasongkit A. Grigoriev, B.Pathak, R. Ahuja and R. Scheicher
Theoretical study of electronic transport through DNA nucleotides in a double-functionalized grapheme nanogap
The Journal of Physical ChemistryC 117, 15421 (2013).

571. R. B. Araujo, R. H. Scheicher, J. S. de Almeida, A.F. da Silva and R.Ahuja
Lithium transport investigations in LixFeSiO4 : a promising cathode material
***Solid State Communication* 173,** 9 (2013).

572. M. Bououdina, Y. Oumellal, L. Dupont, L. Aymard, H. Al-Gharni, A. Al-Hajry, T.A. Maark, A. De Sarkar, R. Ahuja, M.D. Deshpande, Z. Qian, and A.B. Rahane
Lithium storage in amorphous TiNi hydride: electrode for rechargeable lithium-ion batteries
***Materials Chemistry and Physics* 141,** 348 (2013).

573. P. Srepusharawoot, Ekaphan Swatsitang, Vittaya Amornkitbamrung, U. Pinsook and R. Ahuja
Hydrogen Adsorption of Li Functionalized Covalent Organic Framework-366: an Ab Initio Study
***International Journal of Hydrogen Energy* 38,** 14276 (2013).

574. T. Hussain, T. Kaewmaraya, S.Chakraborty and R. Ahuja
Functionalization of hydrogenated silicene with alkali and alkaline earth metals for efficient hydrogen storage
PhysChemChemPhys 15, 18900 (2013).

575. M.Ramzan, Y.G.Li & R.Ahuja
Electronic structure, mechanical and optical properties of In_2O_3 with hybrid density Functional (HSE06)
***Solid State Communications* 172,** 37 (2013).

576. Y-L. Li, W. Luo, X-J. Chen, Z. Zeng, H-Q. Lin & R. Ahuja
Formation of Nanofoam carbon and re-emergence of Superconductivity in compressed CaC_6
***Nature-Scientific Reports* 3,** 3331 (2013).

577. Z. Nabi, S. Amari , S. Méçabih, A. Zaoui , B. Abbar , B. Bouhafs & R. Ahuja
Ferromagnetism in CdOX (X = Mn and N) with and without intrinsic point defects: A density functional theory
***Results in Physics* 3,** 205 (2013).

578. P.Liu, J.Nisar, B. Pathak and R. Ahuja
Cationic–anionic mediated charge compensation on $La2Ti_2O_7$ for visible light photocatalysis
***PhysChemChemPhys* 15,** 17150 (2013)**.**

579. B.C.Wang, P. D. Kanhere, Z. Chen, J.Nisar, B.Pathak and R.Ahuja
Anion Doped $NaTaO_3$ for Visible Light Photocatalysis
***The Journal of Physical ChemistryC* 117,** 22518 (2013).

580. W.Sun, S.Chakraborty & R.Ahuja
Stabilizing a novel hexagonal Ru_2C via Lifshitz transition under pressure
***Appl. Phys. Lett.*103,** 251901 (2013).

581. H. Löfås, R. Emanuelsson, R. Ahuja, A. Grigoriev and H. Ottosson,

Conductance Through Carbosilane Cage Compounds: A Computational Investigation
The Journal of Physical ChemistryC 117, 21692 (2013).

582. T. Hussain, T. A. Maark, B. Pathak and R. Ahuja
Improvement in the hydrogen desorption from MgH_2 upon transition metals doping: A Hybrid Density Functional Calculations
AIP Advances 3, 102117 (2013).

583. C. Århammar, F.Silvearv, A.Bergman, S.Norgren, H.Pedersen & R.Ahuja
A theoretical study of possible point defects incorporated into alpha-alumina deposited by chemical vapor deposition
Theoretical Chemistry Accounts, **133** 1433 (2013).

584. Z. Guo, B. Sa, B. Pathak, J. Zhou, R. Ahuja and Z. Sun
Band gap engineering in huge-gap semiconductor $SrZrO_3$ for visible-light photocatalysis
International Journal of Hydrogen Energy **39,** 2042 (2014).

585. C. Århammar, J.L. Endrino, M. Ramzan, D. Horwat, A. Blomqvist, J-E. Rubensson, J. Andersson and R. Ahuja
Probing temperature-induced ordering in supersaturated Ti1−xAlxN coatings by electronic structure
Surface and Coatings Technology **242,** 207 (2014).

586. T. Hussain, A.D. Sarkar and R. Ahuja
Functionalization of hydrogenated graphene by polylithiated species for efficient hydrogen storage
International Journal of Hydrogen Energy **39**, 2560 (2014).

587. J.C. Lee, J.E. Lee, J.W. Lee, J.Ch. Lee, N.G.Subramaniam, T.W. Kang & R. Ahuja
Se concentration dependent band gap engineering in $ZnO_{1-x}Se_x$ thin film for optoelectronic applications
J. Alloys Compounds **585,** 94 (2014).

588. B.Sa, Z.M.Sun, J.Zhou and R.Ahuja
First-principles investigations of electronic and mechanical properties for stable $Ge_2Sb_2Te_5$ with van der Waals corrections
Computational Materials Science 82, 66 (2014).

589. P.Liu, A.D. Sarkar and R. Ahuja
Shear strain induced indirect to direct transition in band gap in AlN monolayer nanosheet
Computational Materials Science **86,** 206 (2014).

590. Y. Li, R. Ahuja and J. A. Larsson
Origin of the Difference Between Carbon Nanotube Armchair and Zigzag Ends
Journal of Chemical Physics 140, 091102 (2014).

591. W.Sun, T. Hussain, A. D. Sarkar, T. A. Maark, W.Luo & R.Ahuja

Improvement in the desorption of H_2 from the MgH_2 (1 1 0) surface by means of doping and mechanical strain
Computational Materials Science 86, 165 (2014).

592. Z. Qian, X. Jiang, A. D. Sarkar, T. A. Maark, M. D. Deshpande, M. Bououdina, B.Johansson & R. Ahuja
Screening study of light-metal and transition-metal-doped NiTiH hydrides as Li-ion battery anode materials
Solid State Ionics 258, 88 (2014).

593. B. Wang, C. Århammar, X. Jiang, C. M. Araujo and R. Ahuja
A comparison between hybrid functional, GW approach and the Bethe Salpether equation: Optical properties of high pressure phases of TiO_2
Science of Advanced Materials. **6,** 1170 (2014).

594. M.Sagynbaeva, P. Panigrahi , Y. Li, M. Ramzan & R. Ahuja
Tweaking the magnetism of MoS_2 nano ribbon with hydrogen and carbon passivation
Nanotechnology **25,** 165703 (2014) **"Editor Pick".**

595. T. Hussain, P. Panigrahi & R. Ahuja
Enriching Physisorption of H_2S and NH_3 Gases on a Graphane Sheet by doping with Li adatoms
PhysChemChemPhys **16,** 8100 (2014).

596. B. Wang, J. Nisar, C. G. Almeida, A. J. S. Mascarenhas, L. A. Silva, D. G. F. David, P. Bargiela, C. M. Araujo, R. Ahuja and A. F. da Silva
Optical and electronic properties of nanosized $BiTaO_4$ and $BiNbO_4$ photocatalysts: experiment and Theory
Physica Status Solidi B **251** 1034 (2014).

597. R. Emanuelsson, H.Löfås, J. Zhu, R. Ahuja, A.Grigoriev and H. Ottosson,
In Search of Flexible Molecular Wires with Near Conformer-Independent Conjugation and Conductance: A Computational Study
Journal of Physical Chemistry C **118,** 5637 (2014).

598. T. Kaewmaraya, M.Ramzan, J.M.O.Guillen and R.Ahuja
Electronic Structure and Ionic Diffusion of Green Battery Cathode Material: $Mg_2Mo_6S_8$
Solid State Ionics 261, 17 (2014).

599. C. M. Araujo, S. Nagar, M. Ramzan, R. Shukla, O.D. Jayakumar, A.K. Tyagi, Yi-S Liu, J-L Chen, P-A. Glans, C. Chang, A. Blomqvist, R. Lizárraga, E. Holmström, L. Belova, J. Guo, R. Ahuja and K.V.Rao
Disorder-induced Room Temperature Ferromagnetism in Glassy Chromites
Nature-Scientific Reports **4,** 4686 (2014).

600. K.Kotmool, T.Bovornratanaraks and R.Ahuja
High-Pressure Phase Transition of ZnO Nanorods Using Density Functional Theory

Integrated Ferroelectrics.**156,** 122 (2014).

601. T. Kaewmaraya, A.D. Sarkar, B.Sa, Z.Sun & R. Ahuja
Strain-induced tunability of optical and photocatalytic properties of ZnO mono-layer nanosheet
Computational Materials Science **91,** 38 (2014).

602. P.Panigrahi, T. Hussain, C.M. Araujo & R.Ahuja
Hole Induced Jahn Teller Distortion Ensuing Ferromagnetism in Mn-MgO; Bulk, Surface and One dimensional structures
Journal of Physics: Condensed Matter **26,** 265801 (2014).

603. I. Lykissa, S.Y Li, M. Ramzan, S. Chakraborty, R. Ahuja, C. G. Granqvist, and G. A. Niklasson
Electronic density-of-states of amorphous vanadium pentoxide films: Electrochemical data and density functional theory calculations
Journal of Applied Physics **115,** 183701 (2014).

604. Y. Benhouria, I. Essaoudi, A. Ainane, R. Ahuja and F. Dujardin
Dielectric properties and hysteresis loops of a ferroelectric nanoparticle system described by the transverse Ising model
Journal of Superconductivity and Novel Magnetism **27**, 2153 (2014).

605. Y. Benhouria, I. Essaoudi, A. Ainane, R. Ahuja and F. Dujardin
The dielectric properties and the hysteresis loops of the spin-1 Ising nanowire system with the effect of a negative core/shell coupling: A Monte Carlo study
Superlattices and Microstructures **73,** 121 (2014).

606. P.Panigrahi, T. Hussain, C.M. Araujo & R.Ahuja
Crafting Ferromagnetism at Mn doped MgO Surface with p-type Defects
Science and Technology of Advanced Materials **15,** 035008 (2014).

607. Y.Li, Y-L. Li, W.Sun & R.Ahuja
Dynamic stability of the single-layer transition metal diachalcogenides
Computational Materials Science**. 92,** 206 (2014).

608. A.D. Sarkar & R. Ahuja
Electronic charge transport through ZnO nanoribbons
Journal of Physics and Chemistry of Solids.**75,** 1223 (2014).

609. J. Liao, B.Sa, J.Zhou, R. Ahuja and Z. Sun,
Design of High-Efficiency Visible-Light Photocatalysts for Water Splitting: MoS2/AlN(GaN) Heterostructures
Journal of Physical Chemistry C **118,** 17594 (2014).

610. R. Emanuelsson, H. Löfås A.Wallner,D. Nauroozi, J. Baumgartner, C. Marschner, R. Ahuja, S. Ott, A. Grigoriev and H. Ottosson

Configuration- and Conformation-Dependent Electronic-Structure Variations in 1,4-Disubstituted Cyclohexanes Enabled by a Carbon-to-Silicon Exchange
Chemistry - A European Journal **20,** 9304 (2014).

611. B. Wang, M. Lilja, T. Ma, J. Sörensen, H. Stecke, R. Ahuja & M. Strømme
Theoretical and experimental study of the incorporation of tobramycin and strontium- ions into hydroxyapatite by means of co-precipitation
Applied Surface Science **314,** 376 (2014).

612. T. Hussain, P. Panigrahi & R. Ahuja,
Sensing Propensity of a Defected Graphane sheet towards CO, H2O and NO2 gas molecules
Nanotechnology **25**, 325501 (2014).

613. P. D. Kanhere, P.Shenai, S.Chakraborty, R.Ahuja, J.Zheng and Z.Chen
Mono-and co-doped NaTaO3 for visible light photocatalysis
Physical Chemistry Chemical Physics **16,** 16085 (2014).

614. B.Johansson, W.Luo, S. Li & R.Ahuja
Cerium; Crystal Structure and Position in The Periodic Table
Nature-Scientific Reports **4,** 6398 (2014).

615. Y.L. Li, R. Ahuja and H.Q.Lin
Structural phase transition and metallization in compressed SrC_2
Chinese Science Bulletin **59,** 5269 (2014).

616. T. Hussain, S.Chakraborty, A.D. Sarkar, B.Johansson, and R. Ahuja
Enhancement of energy storage capacity of Mg functionalized silicene and silicane under external strain
Appl. Phys. Lett.**105,** 123903 (2014).

617. Y. Benhouria, I. Essaoudi, A. Ainane, R. Ahuja and F. Dujardin,
Thermodynamic properties and hysteresis behaviors of a mixed spin-(3/2) and spin-(1/2) Ising double walled ferrielectric nanotubes: A Monte Carlo study
Superlattices and Microstructures **73,** 121 (2014).

618. P. P. Kong, F. Sun, L.Y. Xing, J. Zhu, S. J. Zhang, W. M. Li, Q. Q. Liu, X. C. Wang, S. M. Feng, X. H. Yu, J. L. Zhu, R. C. Yu, W. G. Yang, G. Y. Shen, Y. S. Zhao, R. Ahuja, H. K. Mao & C. Q. Jin
Superconductivity in Strong Spin Orbital Coupling Compound Sb2Se3
Nature-Scientific Reports **4,** 6679 (2014).

619. K. Kotmool, T. Kaewmaraya, S. Chakraborty, J. Anversa, T. Bovornratanaraks, W. Luo, H. Gou, P. C. Piquini, T. W. Kang, H.K. Mao and R. Ahuja
Revealing an unusual transparent phase of superhard Iron Tetraboride under high pressure
PNAS (the Proceedings of the National Academy of Sciences, USA). **111,** 17050 (2014).

620. B. Sa, Y.L. Li, J. Qi, R. Ahuja and Z. Sun
Strain Engineering for Phosphorene: The Potential Application as a Photocatalyst
Journal of Physical Chemistry C. **118,** 26560 (2014).

621. S. Umrao, S. Abraham, F. Theil, S. Pandey, V. Ciobota, P. K. Shukla, C. J Rupp, S. Chakraborty, R. Ahuja, J. Popp, B. Diezek & A. Srivastava
A Possible Mechanism for the Emergence of Additional Band Gap due to Ti-O-C Bond in TiO2 -Graphene Hybrid System for Enhanced Photodegradation of Methylene Blue under Visible Light
RSC Advances 4, 59890 (2014).

622. H. Löfås, B. O. Jahn, J. Wärnå, R. Emanuelsson, R. Ahuja, A. Grigoriev & H. Ottosson
A Computational Study of Potential Molecular Switches that Exploit Baird's Rule on Excited State Aromaticity and Antiaromaticity
Faraday Discussions **174,** 105 (2014).

623. T.Arslanov, A. Mollaev, I. Kamilov, R. Arslanov, L. Kilanski, R. Minikaev, A. Reszka, S. L. Moreno, A. Romero, M. Ramzan, P. Panigrahi, R. Ahuja, V. Trukhan, T. Chatterji, S. Marenkin, T. Shoukavaya
Pressure control of magnetic clusters in strongly inhomogeneous ferromagnetic chalcopyrites
Nature-Scientific Reports 5, 7720 (2015).

624. S. Bouhou, M. El Hamri, I. Essaoudi, A. Ainane and R. Ahuja
Magnetic properties of a single transverse Ising ferromagnetic nanoparticle
Physica B **456,** 142 (2015).

625. S. Bouhou, I. Essaoudi , A. Ainane, A. Oubelkacem, R. Ahuja and F. Dujardin,
Magnetic properties of a transverse Ising nanoparticle
Journal of Superconductivity and Novel Magnetism **28**, 885 (2015)

626. A. Oubelkacem, I. Essaoudi, A. Ainane, R. Ahuja and F. Dujardin,
The Magnetic Properties of Multi-surface Transverse Ferroelectric Ising Thin Films
Journal of Superconductivity and Novel Magnetism **28**, 877 (2015)

627. T. Hussain, S.Chakraborty, B.Johansson, and R. Ahuja
BC3 Sheet Functionalized with Lithium Rich Species Emerging as a Reversible Hydrogen Storage Material
ChemPhysChem.**16,** 634 (2015).

628. K. Kotmool, T. Bovornratanaraks, S. Chakraborty and R. Ahuja
The effect of morphology and confinement on the high-pressure phase transition in ZnO nanostructure
J. Appl. Phys. **117,** 114309 (2015)

629. M. El Hamri, S. Bouhou, I. Essaoudi, A. Ainane and R. Ahuja
Investigation of the surface shell effects on the magnetic properties of a transverse antiferromagnetic Ising nanocube

***Superlattices and Microstructures* 80**, 151 (2015)

630. X. Zhang, J. Qin, H. Liu, S. Zhang, M. Ma, W. Luo, R. Liu and R. Ahuja
Pressure-induced zigzag phosphorus chain and superconductivity in boron monophosphide
***Nature-Scientific Reports* 5,** 8761 (2015).

631. Rafael B. Araujo, S.Chakraborty and R. Ahuja
Unveiling the charge migration mechanism in Na2O2: A theoretical relevance in sodium air batteries
***PhysChemChemPhys.* 17,** 8203 (2015).

632. F. Silvearv, P.Larsson, S. Jones, R. Ahuja and A. Larsson
Establishing the Most Favorable Metal-Carbon Bond Strength for Carbon Nanotube Catalysts
***J. Mater. Chem. C.* 3,** 3422 (2015).

633. A. Pietzscha, J. Nisar, E. Jämstorp, J. Gråsjö, C. Århammar, R.Ahuja and J.-E. Rubensson
Kaolinite: defect defined material properties -a soft x-ray and first principles study of the band gap
***Journal of electron spectroscopy and related phenomena* 202,** 11 (2015).

634. A. Oubelkacem, I. Essaoudi, A. Ainane, F. Dujardin and R. Ahuja
Effect of Seeding Layers on Hysteresis Loops and Phase Transition of the Ferroelectric Thin Film
***Ferroelectrics* 478,** 1 (2015).

635. R. Johansson, R. Ahuja, O. Eriksson, B. Hjörvarsson, and R. Scheicher
Effect of uniaxial strain on the site occupancy of hydrogen in vanadium from density-functional calculations
***Nature-Scientific Reports* 5,** 10301 (2015).

636. M. Sagynbaeva, T. Hussain, P. Panigrahi, B. Johansson and R. Ahuja
Complementing the adsorption energies of CO_2, H_2S and NO_2 to h-BN sheet by doping with carbon
***Euro Phys. Letters* 109,** 57008 (2015).

637. Q. Lai, A.Thornton, M.Hill, Z. Haung, H.K. Lui., Z. Guo, M.Paskevicius, D. Sheppard, C.Buckely, A. Banerjee, S. Chakraborty, R.Ahuja and K.F. Aguey-Zinsou
Hydrogen storage materials for mobile and stationary applications: Current state of the art
***ChemSusChem* 8,** 2789 (2015).

638. (a) T. Hussain, T. A. Maark, S. Chakraborty and R. Ahuja
Improvement in Hydrogen Desorption from β- and γ-MgH2 on Selected Transition Metal Doping
***ChemPhysChem* 16,** 634 (2015).

(b) Cover page of the issue.

639. Y. Benhouria, I. Essaoudi, A. Ainane and R. Ahuja
Hysteresis behavior and pyroelectric properties of the multi-surface ferroelectric thin films
***Chinese Journal of Physics* 53,** 080802 (2015).

640. (a) T. Hussain, M.Islam, S.G. Rao, P. Panigrahi, D. Gupta and R. Ahuja
Hydrogen Storage Properties of Light Metal Adatoms (Li, Na) Decorated Fluorographene Monolayer
***Nanotechnology* 26,** 275401 (2015).

(b) Nature has mentioned it in their highlights. Please see the following website :

http://www.natureasia.com/en/nindia/article/10.1038/nindia.2015.85

641. M. El Hamri, S. Bouhou, I. Essaoudi, A. Ainane, R. Ahuja and F. Dujardin
Thermodynamic properties of the core/shell antiferromagnetic Ising nanocube
***Journal of Superconductivity and Novel Magnetism* 28,** 3127 (2015).

642. A. Orthaber, H. Löfås, E. Öberg, A. Grigoriev, A. Wallner, M. Santoni, R. Ahuja, K. Leifer, H. Ottosson and S. Ott,
Cooperative Gold Nanoparticle Stabilization by Acetylenic Phosphaalkenes
***Angew. Chem.*127,** 10780 (2015).

643. T. Kaewmaraya, W.Luo, X. Yang, P. Panigrahi and R.Ahuja
A new layered monoclinic phase of Co3O4 at high pressure
***Phys.Chem.Chem.Phys.*17,** 19957 (2015).

644. J. Prasongkit, R. G. Amorim, S. Chakraborty, R. H. Scheicher, R. Ahuja and V. Amornkitbamrung
Highly sensitive and selective gas detection based on silicene
***Journal of Physical Chemistry C* 119,** 16934 (2015).

645. Q.Tay, P. Kanhere, CF. Ng, S. Chen, S. Chakraborty, A. Huan, CT. Sum, R. Ahuja & Z. Chen
Defect Engineered g-C3N4 for Efficient Visible Light Photocatalytic Hydrogen Production
***Chemistry of Materials* 27,** 4930 (2015).

646. C. J. Rupp, S. Chakraborty, R. Ahuja & R. J. Baierle
Impurity effect in ultra-thin hydrogenated silicene and germanene. A first principles study
***Phys.Chem.Chem.Phys.* 17,** 22210 (2015).

647. A. Srivastava, V.Sharma, K.Kaur, R.Ahuja & V.K.Rao
Electron transport properties of a single-walled carbon nanotube in the presence of hydrogen cyanide: first-principles analysis
***JOURNAL OF MOLECULAR MODELING* 21,** 173 (2015).

648. W.Sun, W.Luo & R.Ahuja
Stability of a new cubic monoxide of Thorium under pressure
***Nature-Scientific Reports* 5,** 13740 (2015).

649. D. Dwibedi, R. B. Araujo, S. Chakraborty, P. P. Shanbogh, N. G. Sundaram, R. Ahuja and P. Barpanda
Na2.44Mn1.79(SO4)3: A new member of alluaudite family of insertion compounds for sodium ion batteries
Journal of Materials Chemistry A **3,** 18564 (2015).

650. J. Zhou, B.Sa, Z. Sun, C. Si and R. Ahuja
Manipulating Carriers' Spin Orientation in Heusler Alloy Mn2CoAl
RSC Advances **5,** 73814 (2015).

651. S. H. Jafri, H. Löfås, T. Blom, A. Wallner, A. Grigoriev, R. Ahuja, H. Ottosson, and K. Leifer
Nano-fabrication of molecular electronic junctions by targeted modification of metal-molecule bonds
Nature-Scientific Reports 5, 14431 (2015).

652. Rafael B. Araujo, J. S. de Almeidaa, A. Ferreira da Silva and Rajeev Ahuja
Insights in the electronic structure and redox reaction energy in LiFePO4 battery material from an accurate Tran-Blaha modified Becke Johnson potential
J. Appl. Phys. **118,** 125107 (2015).

653. M. S. Mahabal, M. Deshpande, T. Hussain and R. Ahuja,
Superior sensing characteristics of graphene like boron carbide (BC3) monolayer towards selected toxic gases
ChemPhysChem. **16,** 3511 (2015).

654. I.Choudhuri, N. Patra, A. Mahata, R. Ahuja and B. Pathak
B-N@Graphene: Highly Sensitive and Selective Gas Sensor
Journal of Physical Chemistry C. **119,** 24827 (2015).

655. M. M. Sundaram, T. Watcharatharapong, S. Chakraborty, R. Ahuja, S. Duraisamy, P. T. Rao and N. Munichandraiah
Synthesis, crystal and electronic structure of sodium metal phosphate for hybrid capacitor in non-aqueous electrolyte
Dalton Transactions **44,** 20108 (2015).

656. C. Dahlstrand, B. Jahn, A. Grigoriev, S.Villaume, R. Ahuja and H.Ottosson
Polyfulvenes: Polymers with "Handles" that Enable Extensive Electronic Structure Tuning
Journal of Physical Chemistry C. 119, 25726 (2015).

657. J.Lee, G. Nagarajan, I. A. Kowalik, J. Nisar, J. Lee, Y. Kwon, J. Lee, T. W. Kang, X. Peng, D. Arvanitis, and R. Ahuja
Towards a new class of heavy ion doped magnetic semiconductors for room temperature applications
Nature-Scientific Reports. **5,** 17053 (2015).

658. J. Prasongkit, G. T. Feliciano, A. R. Rocha, Y. He, T. Osotchan, R. Ahuja &

R. H. Scheicher
Theoretical assessment of feasibility to sequence DNA through interlayer electronic tunneling transport at aligned nanopores in bilayer graphene
Nature-Scientific Reports 5, 17560 (2015).

659. P. Kanhere, S. Chakraborty, C. J Rupp, R. Ahuja and Z. Chen
Substitution induced band structure shape tuning in hybrid perovskites (CH3NH3Pb1-xSnxI3) for efficient solar cell applications
***RSC Advances* 5,** 107497 (2015).

660. S. Bouhou, I. Essaoudi, A. Ainane & R. Ahuja
Investigation of a core/shell Ising nanoparticle: thermal and magnetic properties
***Physica B* 481,** 124 (2016).

661. S.G. Rao, T. Hussain, M. Islam, M. Sagynbaeva, D. Gupta, P. Panigrahi and R. Ahuja
Adsorption Mechanism of Graphene like ZnO Monolayer Towards CO2 molecules: Enhanced CO2 Capture
***Nanotechnology* 27,** 015502 (2016).

662. Rafael B. Araujo, M. S. Islam, S. Chakraborty and R. Ahuja
Predicting Electrochemical Properties and Ionic Diffusion in Na2+2xMn2-x(SO4)3: Crafting a Promising High Voltage Cathode Material
***Journal of Materials Chemistry A.* 4**, 451 (2016).

663. Rafael B. Araujo and R. Ahuja
Evaluating bulk Nb2O2F3 for Li-battery electrode application
***Phys.Chem.Chem.Phys.* 18,** 3530 (2016).

664. M. El Hamri, S. Bouhou, I. Essaoudi, A. Ainane and R. Ahuja
Magnetic properties of a diluted spin-1/2 Ising nanocube
***Physica A* 443,** 385 (2016).

665. C. Rupp, S. Chakraborty, J. Anversa, R. Baierle, R. Ahuja,
Rationalizing Hydrogen and Oxygen Evolution Reaction Activity of Twodimensional Hydrogenated Silicene and Germanene,
***ACS Applied Materials and Interfaces,* 8,** 1536 (2016).

666. M. S. Islam, T. Hussain, S.G. Rao, P. Panigrahi and R. Ahuja
Augmenting the sensing Aptitude of Hydrogenated Graphene by Crafting with Defects and Dopants
***Sensors & Actuators: B. Chemical* 228,** 317 (2016).

667. P. Suksaengrat, V. Amornkitbamrung, P. Srepusharawoot and R.Ahuja
Density Functional Theory Study of Hydrogen Adsorption of Ti Decorated Mg-Metal Organic Framework-74
***ChemPhysChem* 17,** 879 (2016).

668. M. El Hamri, S. Bouhou, I. Essaoudi, A. Ainane, R. Ahuja, F. Dujardin
Phase diagrams of a transverse cubic nanowire with diluted surface shell
***Appl. Phys. A* 122,** 202 (2016).

669. D. Dwibedi, C.Ling, R.Araujo, S. Chakraborty, S. Duraisamy, N. Munichandraiah, R. Ahuja, and P. Barpanda
Ionothermal Synthesis of High-voltage Alluaudite Na2+2xFe2-x(SO4)3 Sodium Insertion Compound: Structural, Electronic and Magnetic Insights
***ACS Applied Materials and Interfaces* 8,** 6982 (2016).

670. M. Mahabal, M. Deshpande, S. Chakraborty, T.W. Kang and R.Ahuja,
Rare Earth Functionalization Effect in Optical Response of ZnO Nano Clusters
***Eur. Phys. J. D* 70,** 63 (2016).

671. R. B. Araujo, S. Chakraborty, P. Barpanda and R. Ahuja
Na2M2(SO4)3 (M=Fe, Mn, Co and Ni): Towards High Voltage Sodium Battery Applications
***Phys.Chem.Chem.Phys.* 18,** 9658 (2016).

672. M. El Hamri, S. Bouhou, I. Essaoudi, A. Ainane, R. Ahuja
A theoretical study of the hysteresis behavior of a transverse spin-1/2 Ising nanocube
***Journal of Magnetism and Magnetic Materials* 413,** 30 (2016).

673. N. Ozaki, W. J. Nellis, T. Mashimo, M. Ramzan, R. Ahuja, T. Kaewmaraya, T.Kimura, M. Knudson, K. Miyanishi, Y. Sakawa, T. Sano and R. Kodama
Dynamic compression of dense oxide from 0.4 to 2.6 TPa: Universal Hugoniot of fluid metals
***Nature-Scientific Reports* 6,** 26000 (2016).

674. J. Anversa, S. Chakraborty, P. Piquini and R. Ahuja,
High pressure driven superconducting critical temperature tuning in Sb2Se3 topological insulator
***Appl. Phys. Lett.* 108,** 212601 (2016).

675. M. Minakshi, D. Mitchell, R. Jones, and F. Alenazey, T. Watcharatharapong, S. Chakraborty, and R. Ahuja
Synthesis, structural and electrochemical properties of sodium nickel phosphate for energy storage devices
***Nanoscale* 8,** 11291 (2016).

676. E. Callini, K-F Aguey-Zinsou, R. Ahuja, J. R. Ares, S. Bals, N. Biliškov, S. Chakraborty, G. Charalambopoulou, A-L Chaudhary, F. Cuevas, B. Dam, P. de Jongh, M. Dornheim, Y. Filinchuk, J. G. Novaković, M. Hirscher, T. R. Jensen, P. B. Jensen, N. Novaković, Q. Lai, F. Leardini, D. M. Gattia18, L. Pasquini, T. Steriotis, S. Turner, T. Vegge, A. Züttel, A. Montone
Nanostructured materials for solid-state hydrogen storage: A Review
***International Journal of Hydrogen Energy* 41,** 14404 (2016).

677. P. Banerjee, B. Pathak, R. Ahuja and G.P. Das

First Principles Design of Li Functionalized Hydrogenated
h-BN Nanosheet For Hydrogen Storage
***International Journal of Hydrogen Energy* 41,** 14437 (2016).

678. Y. Benhouria, I. Essaoudi, A. Ainane, R. Ahuja and F. Dujardin
Hysteresis loops and dielectric properties of compositionally graded (Ba,Sr)TiO_3 thin films described by the Transverse Ising Model
***Chinese Journal of Physics* 54,** 533 (2016).

679. S. H. Mir, P. C. Jha , M.S.Islam, A. Banarjee, W. Luo , S. D. Dabhi, P. K. Jha & R.Ahuja
Static and Dynamical Properties of heavy actinide Monopnictides of Lutetium
***Nature-Scientific Reports* 6,** 29309 (2016).

680. D. Singh, S. K. Gupta, Y. Sonavane, A. Kumar and R. Ahuja
2D-HfS2 as an efficient photocatalyst for water splitting
***Catalysis Science & Technology* 6,** 6605 (2016).

681. S. Kumavat, S. Chakraborty, A. B. Rahane, M. D. Deshpande and R.Ahuja
Time Dependent DFT Investigation of Optical Response in Pristine and Gd Doped Al2O3
***RSC Advances.*6,** 72537 (2016).

682. S. Das, D. Dutta, R. Araujo, S. Chakraborty, R. Ahuja and A. Bhattacharyya
Probing the Pseudo-1-D Ion Diffusion in Lithium Titanium Niobate Anode for Li-ion Battery
***Physical Chemistry Chemical Physics* 18,** 22323 (2016).

683. S.H. Mir, S. Chakraborty, P.C. Jha, J.Warna, H. Soni, P.K.Jha and R.Ahuja,
Two-dimensional Boron: Lightest Catalyst for Hydrogen and Oxygen Evolution Reaction
***Appl. Phys. Lett.*109,** 053903 (2016).

684. H Shi, T. Hussain, R. Ahuja, T. W. Kang, and W. Luo
Role of vacancies, light elements and rare-earth metals doping in CeO2
***Nature-Scientific Reports* 6,** 31345 (2016).

685. S. Höfner, S. Bladh, B. Aringer and R. Ahuja
Dynamic atmospheres and winds of cool luminous giants I. Corundum and silicate dust in the close vicinity of M-type AGB stars
***Astronomy & Astrophysics* 594,** A108 (2016).

686. K. Kotmool, B. Li, S. Chakraborty, T. Bovornratanaraks, W. Luo, Ho-kwang Mao and R. Ahuja,
High pressure induced distortion in face-centered cubic phase of thallium
PNAS 113, 11143 (2016).

687. M. Manasi ; M. Deshpande, T. Hussain and R. Ahuja,
Sensing Characteristics of Phosphorene Monolayers Towards PH3 and AsH3 Gases Upon the Introduction of Vacancy Defects

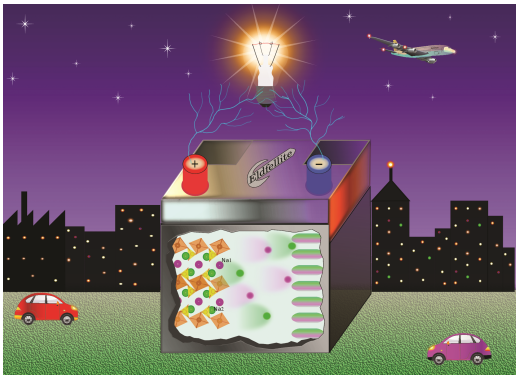
***The Journal of Physical Chemistry C* 120,** 20428 (2016).

688. K. Kotmool, T. Bovornratanaraks, U.Pinsook and R. Ahuja,
Superhard Semiconducting Phase of Osmium Tetraboride Stabilizing at 11 GPa
The Journal of Physical Chemistry C 120, 23165 (2016).

689. C. A. Triana, C. Moyses Araujo, R. Ahuja, G.Niklasson and T.Edvinsson
Electronic transitions induced by short-range structural order in amorphous TiO2
***Physical Review B.* 94,** 165129 (2016).

690. M. El Hamri, S. Bouhou, I. Essaoudi, A. Ainane, R. Ahuja and F. Dujardin
Some characteristic behaviors of a spin-1/2 Ising nanoparticle
Journal of Physics: C. 758 012023 (2016).

691 (a). A.Banerjee, R. Araujo and R.Ahuja
Unveiling the Thermodynamic and Kinetic Properties of Eldfellite, NaFe(SO4)2: Toward a High-capacity and Low-cost Cathode Material
***Journal of Materials Chemistry A* 4,** 17960 (2016).



691 (b). Issue's cover page.

692. M. El Hamri, S. Bouhou, I. Essaoudi, A. Ainane, R. Ahuja
Magnetic properties of a diluted transverse spin-1 ising nanocube with a longitudinal crystal-field
***Proc. SPIE* 10174**, 1017409 (2016).

693. T. Hussain, T. Kaewmaraya, S. Chakraborty and R. Ahuja
Defect and Substitution Induced Silicene Sensor to Probe Toxic Gases
***The Journal of Physical Chemistry C* 120,** 25256 (2016).

694. Y. Benhouria, A. Oubelkacem, I. Essaoudi, A. Ainane and R. Ahuja
Dynamic Magnetic Properties of a Mixed Spin Ising Double-Walled Ferromagnetic Nanotubes: A Dynamic Monte Carlo Study
***Journal of Superconductivity and Novel Magnetism* 30,** 839 (2017).

695. D. Dwibedi, R. Gond, A. Dayamani, R. B. Araujo, S. Chakraborty, R. Ahuja and P. Barpanda
Na2.32Co1.84(SO4)3 as a New Member of Alluaudite Family of High-Voltage Sodium

Battery Cathode
Dalton Transactions, 46, 55 (2017).

696 (a). Y. Li, Y-L Li, B. Sa and R. Ahuja
Review of two-dimensional materials for photocatalytic water splitting from a theoretical perspective
Catalysis Science & Technology **7,** 545 (2017).

696 (b). Issue's cover page.

697. M. El Hamri, S. Bouhou, I. Essaoudi, A. Ainane, R. Ahuja and F. Dujardin
Magnetic behaviors of a transverse spin-1/2 Ising cubic nanowire with core/shell structure
Physica B **507,** 51 (2017).

698. A. Jain, A. Jain, S. Panwar, R. Singh, M. Singhal, J.K Sharma, R. Ahuja, H.C Jeon, T.W Kang, S. kumar
Studies of hypro-mellose(HPMC) functionalized ZnS:Mn fluorescent quantum dots
Journal of Materials Science: Materials in Electronics **28,** 1931 (2017).

699. S. R. Naqvi, G. S. Rao, W. Luo, R. Ahuja and T. Hussain
Hexagonal Boron Nitride (h-BN) sheets decorated with OLi, ONa and Li2F molecules for enhanced energy storage
ChemPhysChem **18,** 513 (2017).

700. R. B. Araujo, A. Banerjee, P. Panigrahi, L. Yang, M. Sjödin, M. Strømme, C. M. Araujo and R. Ahuja
Assessing Electrochemical Properties of Polypyridine and Polythiophene for Prospective Application in Sustainable Organic Batteries
Phys.Chem.Chem.Phys. **19,** 3307 (2017).

701. Z. Qian, H. Raghubanshi, M. Sterlin Leo Hudson, O. N. Srivastava and R. Ahuja
Atomic and electronic exposure of graphene nanofibers to facilitate hydrogen release of hydrazine borane
Chemical Physics Letters **669,** 110 (2017).

702. S.H. Mir, S. Chakraborty, J.Warna, S.Narayan, P.C. Jha, P.K.Jha and R.Ahuja
A Comparative Study of Hydrogen Evolution Reaction on WS2 and PtS2 pseudo-monolayer: Insight based on Density Functional Theory
***Catalysis Science & Technology* 7,** 687 (2017).

703. R. B. Araujo, A. Banerjee, P. Panigrahi, L. Yang, M. Strømme, M. Sjödin, C. M. Araujo and R. Ahuja
Designing strategies to tune reduction potential of organic molecules for sustainable high capacity batteries application
***Journal of Materials Chemistry A* 5,** 4430 (2017).

704. S. R. Naqvi, T. Hussain, P. Panigrahi, W. Luo and R. Ahuja
Manipulating Energy Storage Characteristics of Ultrathin Boron Carbide Monolayer Under Varied Scandium Doping
***RSC Advances* 7,** 8598 (2017).

705. K. Kotmool, S. Chakraborty, T. Bovornratanaraks and R. Ahuja,
Role of relativity in high pressure phase transitions of thallium
***Nature-Scientific Reports* 7,** 42983 (2017).

706. K. Htoutou1, A. Oubelkacem, Y. Benhouria, I. Essaoudi, A. Ainane and R. Ahuja
The magnetic properties of the mixed ferrimagnetic Ising system with random crystal field
Journal of Superconductivity and Novel Magnetism 30, 1247 (2017).

707. Cheng Ji, Alexander F. Goncharov, Vivekanand Shukla, Naresh K. Jena, Dmitry Popov, Bing Li, Junyue Wang, Yue Meng, Vitali Prakapenka, Jesse S. Smith, Rajeev Ahuja, Wenge Yang and Ho-Kwang Mao
Stability of Ar(H2)2 to 358 GPa
PNAS (the Proceedings of the National Academy of Sciences, USA) 114, 3596 (2017).

708. W. Sun, W. Luo, Q. Feng and R. Ahuja
Anisotropic distortion and Lifshitz transition in alpha -Hf under pressure
Physical Review B. 95, 115130 (2017).

709. S. Chakraborty, W. Xie, N.Mathews, M. Sherburne, R. Ahuja, M. Asta and S.Mhaisalkar
Rational Design - A High-Throughput Computational Screening and Experimental Validation Methodology for Lead-free and Emergent Hybrid Perovskites
ACS Energy Letters (Invited Perspective), 2, 837 (2017).

710. O. Parlak, Y. K. Mishra, A. Grigoriev, M. Mecklenburg, W. Luo, S. Keene, A. Salleo, K. Schulte, R. Ahuja, R. Adelung, A. P. F. Turner and A. Tiwari
Hierarchical Aerographite Nano-Microtubular Tetrapodal Networks based Electrodes as Lightweight Supercapacitor
Nano Energy 34, 570 (2017).

711. S.R. Naqvi, T. Hussain, W.Luo and R. Ahuja

Exploring Doping Characteristics of Various Adatoms on Single-layer Stanene
The Journal of Physical Chemistry C, **121,** 7667 (2017).

712. Y. Benhouria, I. Essaoudi, A. Ainane, R. Ahuja and F.Dujardin
Monte Carlo simulation of dielectric properties of a mixed spin-3/2 and spin-5/2 Ising ferrielectric nanowires
Ferroelectrics **507,** 58 (2017).

713. R. Gond, S. Meena, S. Yusuf, V. Shukla, N. Jena, R. Ahuja, S.Okada, P. Barpanda,
Enabling the Electrochemical Activity in Sodium Iron Metaphosphate
[NaFe(PO3)3] Sodium Battery Insertion Material: Structural and Electrochemical Insights
Inorganic Chemistry **56,** 5918 (2017).

714. V. Ragupathi, M. Safiq, P. Panigrahi, T. Hussain, S. Raman, R. Ahuja and G. S. Nagarajan
Enhanced electrochemical performance of LiMnBO3 with conductive glassy phase: a prospective cathode material for lithium-ion battery
Ionics 23, 1645 (2017).

715. C. Triana, C. Araujo, R. Ahuja, G. Niklasson, and T. Edvinsson
Disentangling the intricate atomic short-range order and electronic properties in amorphous transition metal oxides
Nature-Scientific Reports **7,** 2044 (2017).

716. D. Long, M. Li, M. Luo, J. Zhu, H. Yang, Z-B. Huang, R. Ahuja and Y. He
Theoretical investigation on thermodynamic properties of ZnO1-xTex alloys
Materials Research Express **4,** 055901 (2017).

717. X. Yang, H. Li, R. Ahuja, T.W Kang, and W. Luo
Formation and electronic properties of palladium hydrides and palladium-rhodium dihydride alloys under pressure
Nature-Scientific Reports **7,** 3520 (2017).

718. N. Jena, R. Araujo, V.Shukla and R. Ahuja
Borophane as a Bench-mate of Graphene: A Potential 2D Material for Anode of Li and Na-ion Batteries
ACS Applied Materials & Interfaces 9, 17977 (2017).

719. T. Watcharatharapong, M. Minakshi Sundaram, S. Chakraborty, D. Li, G.M. Shafiullah, R.D. Aughterson and R. Ahuja,
Effect of transition metal cations on stability enhancement for molybdate based hybrid supercapacitor
ACS Applied Materials & Interfaces **9,** 16148 (2017).

720. M. El Hamri, S. Bouhou, I. Essaoudi, A. Ainane and R. Ahuja
Reentrant phenomenon in a transverse spin-1 Ising nanoparticle with diluted magnetic sites
Journal of Magnetism and Magnetic Materials **442,** 53 (2017).

721. M. Li, D.Long, R. Ahuja and Y. He
Magnetic Order and Phase Diagram of Magnetic Alloy System: MgxNi1-xO alloy
***Physica Status Solidi B: Basic Solid State Physics* 254,** 1700085 (2017).

722. J.Li and R.Ahuja
Unsaturated surface in CO saturation
***Surface and Interface Analysis* 49,** 892 (2017).

723. V. Singh, V. Kumar, U. Yadav, R. K. Srivastava, V.N. Singh, A. Banerjee, S. Chakraborty, A. K. Shukla, D. K. Misra, R. Ahuja, A. Srivastava and P. S. Saxena
Sensitive and selective detection of copper ions using low cost nitrogen doped carbon quantum dots as a fluorescent sensing plateform
ISSS J Micro Smart Syst. 6, 109 (2017).

724. R. Araujo, A. Banerjee and R. Ahuja,
Divulging the Hidden Capacity and Sodiation Kinetics of $Na_xC_6Cl_4O_2$: A High Voltage Organic Cathode for Sodium Rechargeable Batteries
***The Journal of Physical Chemistry C* 121,** 14027 (2017).

725. A. Bouibes, A.Zaoui, W. Luo and R. Ahuja
Promising optical characteristics of zinc peroxide from first-principles investigation
***Solid State Comunications* 263,** 6 (2017).

726. D. Singh, S.Gupta, Y. Sonvane and R. Ahuja
High performance material for hydrogen storage: graphenelike Si2BN solid
***International Journal of Hydrogen Energy* 36,** 22942 (2017).

727. A. Chafai, I. Essaoudi, A. Ainane, F. Dujardin and R. Ahuja
Tuning the binding energy of on-center donor in CdSe/ZnTe core/shell quantum dot by the spatial parameters and the magnetic field strength
***Physica E* 94,** 96 (2017).

728. A. Chafai, I. Essaoudi, A. Ainane, R. Ahuja and F. Dujardin
Shallow donor inside core/shell spherical nanodot: effect of nanostructure size and dielectric environment on energy spectrum
***Superlattices and Microstructures* 111,** 976 (2017).

729. T. Hussain, T. Kaewmaraya, M.Khan, S.Chakraborty, M. Islam, V. Amornkitbamrung and R. Ahuja,
Improved Sensing Characteristics of Methane over ZnO Nano Sheets Upon Implanting Defects and Foreign Atoms Substitution
***Nanotechnology* 28,** 415502 (2017).

730. M. El Hamri, S. Bouhou, I. Essaoudi, A. Ainane, R. Ahuja and F. Dujardin
Hysteresis loop behaviors of a decorated double-walled cubic nanotube

***Physica B* 524,** 137 (2017).

731. A. Banerjee, S. Chakraborty and R. Ahuja,
Bromination Induced Stability Enhancement with Multivalley Optical Response Signature in Guanidinium [C(NH2)3]+ Based Hybrid Perovskite Solar Cells
***Journal of Materials Chemistry A.* 5,** 18561 (2017).

732. P. Wang, X. Jiang, J. Hu, X. Huang, J. Zhao and R. Ahuja,
Prediction of huge magnetic anisotropies in 5d transition metallocenes
***Journal of Physics : Condensed Matter* 29,** 435802 (2017).

733. I. Essaoudi, M. El Hamri, A. Ainane, F. Dujardin, S. Bouhou and R. Ahuja
Some hysteresis loop features of 2D magnetic spin-1 Ising nanoparticle: shape lattice and single-ion anisotropy effects
***Chinese Journal of Physics* 55,** 2224 (2017).

734. Sh.U. Yuldashev, Z.A. Yunusov, Y.H. Kwon, S.H. Lee, R. Ahuja and T.W. Kang
Critical behavior of the resistivity of GaMnAs near the Curie temperature
***Solid State Comunications* 263,** 38 (2017).

735. V. Shukla, R. Araujo, N. Jena and R. Ahuja
The Curious Case of Two Dimensional Si2BN: A High-capacity Battery Anode Material
***Nano Energy* 41,** 251 (2017).

736. T. Watcharatharapong, J. T-Thienprasert, P. Barpanda, R. Ahuja and S. Chakraborty
Mechanistic study of Na-ion diffusion and small polaron formation in Kröhnkite Na2Fe(SO4)2·2H2O based cathode materials
***Journal of Materials Chemistry A* 5,** 21726 (2017).

737. Z. Qian, W. Guo, G. Jiang, S. Xu, R. Ahuja and X.Liu
Revisiting Mg-Mg2Ni System from Electronic Perspective
***Metals* 7,** 489 (2017).

738. V. Shukla, N. Jena, A. Grigoriev and R. Ahuja
Prospects of Graphene-hBN Heterostructure Nanogap for DNA Sequencing
***ACS Applied Materials & Interfaces* 9,** 39945 (2017).

739. V. Shukla, J. Wärnå, N. Jena, A. Grigoriev and R. Ahuja
Towards the Realization of 2D Borophene Based Gas Sensor
***J. Phys. Chem. C* 121,** 26869 (2017).

740. B. Philippe, T. J. Jacobsson, J. Correa-Baena, N. Jena, A.Banerjee, S. Chakraborty, U. Cappel, R. Ahuja, A. Hagfeldt, M.Odelius and H. Rensmo
Valence Level Character in a Mixed Perovskite Material and Determination of the Valence Band Maximum from Photoelectron Spectroscopy: Variation with Photon Energy
***J. Phys. Chem. C* 121,** 26651(2017).

741. M. Minakshi, T. Watcharatharapong , S. Chakraborty and R. Ahuja
A combined theoretical and experimental approach of a new ternary metal oxide in molybdate composite for hybrid energy storage capacitors
***APL Materials* 6,** 047701 (2018).

742. S. Shi, L. Zhu, H. Zhang, Z.Sun and R. Ahuja,
Mapping the relationship among composition, stacking fault energy and ductility in Nb alloys: a first-principles study
***Acta Materialia* 144,** 853 (2018).

743. T. Hussain, H. Vovusha, T. Kaewmaraya, V. Amornkitbamrung and R. Ahuja
Adsorption Characteristics of DNA Nucleobases, Aromatic Amino Acids and Heterocyclic Molecules on Silicene and Germanene Monolayers
***Sensors & Actuators: B. Chemical* 255,** 2713 (2018).

744. R.Almeida, A. Banerjee, S. Chakraborty, J.Almeida and R. Ahuja
Theoretical Evidences Behind Bifunctional Catalytic Activity in Pristine and Functionalized Al2C monolayer
***ChemPhysChem* 19,** 148 (2018).

745. X. Yang, H. Li, M. Hu, Z. Liu, J. Wärnå, R. Ahuja, Yuying Cao and W.Luo
Mechanical properties of single-wall ZrO2 nanotubes: A finite element approach
***Physica E* 98,** 23 (2018).

746. T. Ouyanga, Z. Qian, R. Ahuja and X. Liu
First-principles investigation of CO adsorption on pristine, C-doped and N-vacancy defected hexagonal AlN nanosheets
***Applied Surface Science* 439,** 196 (2018).

747. C.A. Triana, C. M. Araujo, R. Ahuja, G.A. Niklasson, and T. Edvinsson
Modeling of Electronic Properties of Amorphous Oxides
***Wandelt, K., (Ed.) Encyclopedia of Interfacial Chemistry: Surface Science and Electrochemistry,* vol. 6,** 319–331 (2018).

748. A. Oubelkacem, Y. Benhouria, I. Essaoudi, A. Ainane and R. Ahuja
The magnetic properties and hysteresis behaviors of the mixed spin (½,1) ferrimagnetic nanowire
***Physica B* 549,** 82 (2018).

749. S.R. Naqvi, T. Hussain, W.Luo and R. Ahuja
Metallized Siligraphene Nanosheets (SiC7) as High Capacity Hydrogen Storage Materials
***Nano Research* 11,** 3802 (2018).

750. S. Das, D.Swain, R. Araujo, S. Shi, R. Ahuja, T. Guru Row and A. Bhattacharyya
Alloying in an intercalation host: An alternative chemical design strategy of anodes for rechargeable alkali-ion batteries

Chemistry - An Asian Journal 13, 299 (2018).

751. K. Pandey, D. Singh, S. K. Gupta, P. Yadav, Y. Sonvane, MN. Kumar, I. Lukacevic, M. Kumar and R. Ahuja
Improvements in the hybrid perovskite solar cells with CaMnO3-based electron transport layer
NanoEnergy 45, 287 (2018).

752. A. Srivastava, Md. S. Khan and R. Ahuja
Electron Transport in NH3/NO2 Sensed Buckled Antimonene
***Solid State Comunications* 272,** 1 (2018).

753. P. Tsuppayakorn-aek, W. Luo, R. Ahuja amd T. Bovornratanaraks
The High-Pressure Superconducting phase of Arsenic
Nature-Scientific Reports 8, 3026 (2018).

754. P. Panigrahi, S. R. Naqvi, M. Hankel, R. Ahuja and T. Hussain
Enriching the Hydrogen Storage Capacity of Carbon Nanotube Doped with Polylithiated Molecules
***Applied Surface Science* 444,** 467 (2018).

755. P. Jimlim, K. Kotmool, U. Pinsook, S. Assabumrungrat, R. Ahuja and T. Bovornratanaraks
Theoretical aspects in structural distortion and electronic properties of lithium peroxide under high pressure
***Phys.Chem.Chem.Phys.* 20,** *9488* (2018).

756. A. Banerjee, R. Araujo, M. Sjödin and R. Ahuja
Identifying the Tuning Key of Disproportionation Redox Reaction in Terephthalate: A Li-based Anode for Sustainable Organic Batteries
***NanoEnergy* 47,** 301 (2018). (Cover picture)

757. D. Long, M. Li, D. Meng, R. Ahuja and Y. He
Theoretical investigation of the structural, electronic, and thermodynamic properties of CdS1-xSex alloys
***J.Appl. Phys.* 123,** 105103 (2018).

758. A. Chafai, I. Essaoudi, A. Ainane, F. Dujardin and R. Ahuja,
Recombination energy for negatively charged excitons inside type-II core/shell spherical quantum dots
***Physica E* 101,** 125 (2018).

759. G. Jiang, Z. Qian, M. Bououdina, R. Ahuja and X. Liu
Exploring pristine and Li-doped Mg2NiH4 compounds with potential lithium-storage properties: Ab initio insight
***J. Alloys & Compounds* 746,** 140 (2018).

760. P. Tsuppayakorn-aek, W. Luo, T. Watcharatharapong, R. Ahuja amd T. Bovornratanaraks
Structural prediction of host-guest structure in lithium at high pressure

***Nature-Scientific Reports* 8,** 5238 (2018).

761. K. Cheng, Y. Guo, N. Han, X. Jiang, J. Zhang, R. Ahuja, Y. Su, and J. Zhao
2D lateral heterostructures of group-III monochalcogenide: Potential photovoltaic applications
***Appl. Phys. Lett.* 112,** 143902 (2018).

762. A. Chafai, I. Essaoudi, A. Ainane, F. Dujardin and R. Ahuja,
ZnTe/CdSe type-II core/shell spherical quantum dot under an external electric field
Materials and Devices 3, 0504 (2018).

763. T. Hussain, T. Kaewmaraya, S. Chakraborty, H.Vovusha, V. Amornkitbamrung, and R. Ahuja
Defected and Functionalized Germanene based Nanosensors under Sulfur Comprising Gas Exposure
***ACS Sensors* 3,** 867 (2018).

764. S. K. Kwon, Y. M. Koo, J.-Y. Lee, M. Punkkinen, S. Schoenecker, Z. Nabi, K. Kádas, V. Zólyomi, QM. Hu, R. Ahuja, B. Johansson, J. Kollár and L.Vitos
The surface energy and stress of metals
***Surface Science* 674,** 51 (2018).

765. Y. Benhouria, I. Bouziani, I. Essaoudi, A. Ainane and R. Ahuja
Quantum Monte Carlo study of dynamic magnetic properties of nano-graphene
***J. Magn. Mag. Materials* 460,** 223(2018).

766. D. Saraf, S. Chakraborty, A.Kshirsagar and R.Ahuja
In Pursuit of Bifunctional Catalytic Activity in PdS2 pseudo-monolayer through Reaction Coordinate Mapping
***NanoEnergy* 49,** 283 (2018).

767. J. Li, X. Heb, C. Peng and R. Ahuja
Chemical Bonding of Unique CO on Fe(100)
***J.Phys.Chem.C*. 122,** 9062 (2018).

768. D. Smazna, S. Shree, J. Rodrigues, V. Postica, G. Neubüser, A. F. Ben Sedrine, N. K. Jena, L. Siebert, F. Schütt, O. Lupan, R. Ahuja, M. R. Correia, T. Monteiro, L. Kienle, Y. Yang, R. Adelung, Y. K. Mishra
Buckminsterfullerene Hybridized Zinc Oxide Tetrapods: Defects and Charge Transfer Induced Optical and Electrical Response
Nanoscale 10, 10050 (2018).

769. P. Panigrahi, A. Dhinakaran, Y. Sekar, R. Ahuja and T. Hussain
Efficient Adsorption Characteristics of Pristine and Silver Doped Graphene-Oxide Towards Contaminants: A Novel Approach To Water Purification Mechanism
***ChemPhysChem* 19,** 2250(2018).

770. Y. Benhouria, I. Essaoudi, A. Ainane, R. Ahuja and F. Dujardin
Hysteresis loops and dielectric properties of a mixed spin Blume–Capel Ising ferroelectric nanowire
***Physica A* 506,** 499 (2018).

771. P. Panigrahi, A.K.Dhinakaran, S.R.Naqvi, S.G. Rao, R. Ahuja and T. Hussain
Light Metal Decorated Graphdiyne (GDY) Nanosheets for Reversible Hydrogen Storage
***Nanotechnology* 29,** 355401 (2018).

772. S. Chakraborty, A. Banerjee, T. Watcharatharapong, R. Araujo and R. Ahuja
Current Computational Trends in Polyanionic Cathode Materials for Li and Na batteries
Topical Review *in Journal of Physics: Condensed Matter.*30, 283003 (2018).

773. R. Belghit, H. Belkhir, M. T. Kadri, D. Heciri, M. Bououdina and R. Ahuja
Structural, elastic, electronic and optical properties of newly antiferroelectric KNaX (X= S, Se, and Te) compounds: First principles study
***Physica B* 545,** 18 (2018).

774. T. Hussain, H. Vovusha, R. Umer and R. Ahuja
Superior Sensing Affinities of Acetone Towards Vacancy Induced and Metallized ZnO Monolayers
***Applied Surface Science* 456,** 711 (2018).

775. S. Kansara, S. K. Gupta, Y. Sonvane, T. Hussain and R. Ahuja
Theoretical Investigation of Metallic Nanolayers For Charge-Storage Applications
***Applied Energy Materials* 1,** 3428 (2018).

776. M. Behloul, Y. Benhouria, I. Essaoudi, A.Ainane, H. Ez-Zahraouy and R. Ahuja
Ferromagnetism induced by Cr, V single and double impurities doped BN from Ab-initio and Monte Carlo study
***Computational Condensed Matter* 16,** e00317 (2018).

777. N. Djouambi,C. Bougheloum , A. Messalhi , M. Bououdina, A. Banerjee , S. Chakraborty and R. Ahuja
New Concept on Photocatalytic Degradation of Thiophene Derivatives: Experimental and DFT Studies
***J. Phys. Chem. C* 122,** 15646 (2018).

778. R. Belghit, H. Belkhir, D. Heciri, M.T. Kadri, M. Bououdina and R. Ahuja,
First principles study of structural, mechanical and electronic properties of the ternary alkali metal oxides KNaO and RbNaO
***Chemical Physics Letters* 706,** 684 (2018).

779. T.Hussain, H.Vovusha, T. Kaewmaraya, A. Karton, V. Amornkitbamrung and R. Ahuja
Graphitic Carbon Nitride Nano Sheets Functionalized With Selected Transition Metal Dopants: An Efficient Way To Store CO2

***Nanotechnology* 29,** 415502 (2018).

780. I. Bouziani, Y. Benhouria, I. Essaoudi, A. Ainane and R. Ahuja
Magnetoelectronic properties of Vanadium impurities co-doped (Cd, Cr)Te compound for spintronic devices: First principles calculations and Monte Carlo simulation
***J. Magn. Mag. Materials* 466,** 420 (2018).

781. T. Ouyang, Z. Qian, X. Hao, R. Ahuja and X. Liu,
Effect of Defects on Adsorption Characteristics of AlN Monolayer towards SO2 and NO2: Ab initio Exposure
***Applied Surface Science* 462,** 615 (2018).

782. D. Singh, S. K. Gupta, Y. Sonvane, T. Hussain and R. Ahuja
Achieving ultrahigh carrier mobilities and opening the band gap in two-dimensional Si2BN
***Physical Chemistry Chemical Physics* 20,** 21716 (2018).

783. N. T.Tien, V.T. Phuc and R.Ahuja
Tuning electronic transport properties of zigzag graphene nanoribbons with silicon doping and phosphorus passivation
***AIP Advances* 8,** 085123 (2018).

784. A. Chafai, I. Essaoudi, A. Ainane, F. Dujardin and R. Ahuja
Hydrogenic donor in a CdSe/CdS quantum dot: effect of electric field strength, nanodot shape and dielectric environment on the energy spectrum
***Physica E.* 104,** 29 (2018).

785. A. Banerjee, S. Chakraborty, N.Jena and R. Ahuja
Scrupulous Probing of Bifunctional Catalytic Activity of Borophene Monolayer: Mapping Reaction Coordinate with Charge Transfer
***Applied Energy Materials* 1,** 3571 (2018).

786. X. Zhao, J. Hu, B. Wu, A. Banerjee, S. Chakraborty, J. Feng, Z-Y. Zhao, S. Chen, R.Ahuja, T.C. Sum and Z. Chen
Simultaneous enhancement in charge separation and onset potential for water oxidation in BiVO4 photoanode by W-Ti cooping
***Journal of Materials Chemistry A* 6,** 16965 (2018).

787. V. Shukla, R.B.Araujo, N.Jena and R. Ahuja
Borophene's Tryst with Stability: Exploring 2D Hydrogen Boride as Electrode for Rechargeable Batteries
***Physical Chemistry Chemical Physics* 20,** 22008(2018).

788. X. Yang, W. Luo, Y. Cao, C. Fan, X. Liang, R. Ahuja and H. Li
Corrigendum to "Mechanical stability and formation analysis of Pd/Rh dihydride alloys under pressure" [Solid State Commun. 277 (2018) 33-38]
***Solid State Commun.* 283,** 52 (2018).

789. I. Bouziani, Y. Benhouria, M. Bahloul, I. Essaoudi, A. Ainane and R. Ahuja
Magnetoelectronic properties of GaN codoped with (V, Mn) impurities: Ab-initio and Monte-Carlo studies
***Physica A* 512,** 1249 (2018).

790. D. Long, M. Li, D. Meng, Y. He, I. T. Yoon, R. Ahuja and W. Luo
Accounting for the thermo-stability of PdHx (x = 1–3) by density functional theory
***Int. J. Hydrogen Energy* 43,** 18372 (2018).

791. R. Manotum, R. Klinkla, U. Pinsook, K.Kotmool, P Tsuppayakorn-ak, R.Ahuja and T. Bovornratanaraks,
Effect of pressure on the structure stability, electronic structure and band gap engineering in $Zn_{16}O_1S_{15}$
Computational Condensed Matter 16, e00332 (2018).

792. V. Shukla, A. Grigoriev, N. Jena and R. Ahuja
Strain controlled electronic and transport anisotropy in two-dimensional borophene sheets
***Physical Chemistry Chemical Physics* 20,** 22952 (2018).

793. S. Kumar, V. K. Magotra, H.C. Jeon, T.W. Kang, A. I. Inamdar, A. T. Aqueel, H. Im and R. Ahuja
Multifunctional ammonium fuel cell using compost as a novel electro-catalyst
***Journal of Power Sources* 402,** 221 (2018).

794. D. Heciri, H. Belkhir, A. Hamidani, M. Bououdina and R. Ahuja
Theoretical Investigation of Structural, Electronic and Optical Properties of $(BeS)_1/(BeSe)_1$, $(BeSe)_1/(BeTe)_1$ and $(BeS)_1/(BeTe)_1$ Superlattices under Pressure
***Chemical Physics Letters* 713,** 71 (2018).

795. P. Tsuppayakorn-aek, W. Luo, W. Pungtrakoon, K. Chuenkingkaew, T. Kaewmaraya, R. Ahuja and T. Bovornratanaraks,
The ideal commensurate value of Sc and the superconducting phase under high pressure
***J. Appl. Phys.* 124,** 225901 (2018).

796. T. Hussain, D. Singh, S. K. Gupta, A. Karton, Y. Sonvane and R. Ahuja
Efficient and Selective Sensing of Nitrogen Containing Gases by Si_2BN Nanosheets Under Oxygen Rich Conditions
***Appl. Surface Science* 469,** 775 (2019).

797. K. Klaa, S. Labidi, A. Banerjee, S. Chakraborty, M. Labidi, A. Amara, M. Bououdina and R. Ahuja
Composition Dependent Tuning of Electronic and Magnetic Properties in Transition Metal Substituted Rock-Salt MgO
***J. Magn. Mag. Materials* 475,** 44 (2019).

798. Y. Benhouria, N. Khossossi, M. Houmad, I. Essaoudi, A. Ainane and R. Ahuja
Dynamic magneto-caloric effect of a multilayer nanographene: Dynamic quantum Monte Carlo
Physica E. **105,** 139 (2019).

799. M. Houmad, I. Essaoudi, A. Ainane, A. El Kenz, A. Benyoussef and R. Ahuja
Improving the electrical conductivity of Siligraphene SiC7 by strain
Optik (Optics) **177,** 118 **(2019).**

800. M. Meenakshi, D. Mitchell, C. Baur, J. Chable, A. Barlow, M. Fichtner, A. Banerjee, S. Chakraborty and R. Ahuja,
Phase evolution in calcium molybdate nanoparticles as a function of synthesis temperature and its electrochemical effect on energy storage
Nanoscale Advances **1,** 565 (2019).

801 (a). T. Watcharatharapong, J. T-Thienprasert, S. Chakraborty, and R. Ahuja,
Defect formations and pH-dependent kinetics in kröhnkite Na2Fe(SO4)2·2H2O based cathode for sodium-ion batteries: Resembling synthesis conditions through chemical potential landscape
NanoEnergy **55,** 123 (2019).

801 (b). Cover picture of the issue.

802. A. Chafai, I. Essaoudi, A. Ainane, F. Dujardin and R. Ahuja
Role of a uniform magnetic field on the energy spectrum of a single donor in a core/shell spherical quantum dot
Chinese Journal of Physics **57,** 189 (2019).

803. Y. Benhouria, I. Essaoudi, A. Ainane and R. Ahuja
Dynamic magneto-caloric effect of a C70 Fullerene: Dynamic Monte Carlo
Physica E **108,** 191 (2019).

804. I. Bouziani, Y. Benhouria, I. Essaoudi, A. Ainane and R. Ahuja
Half-metallic ferromagnetic behavior in (Ga, Cr)N and (Ga, Cr, V)N compounds for spintronic technologies: Ab-initio and Monte Carlo methods
Journal of Magnetism and Magnetic Materials **477,** 220 (2019).

805. T. Das, S. Chakraborty, R. Ahuja and G. P. Das
TiS2 Monolayer Emerging as Ultrathin Bifunctional Catalyst : Influence of Defect and Functionalization
ChemPhysChem **20,** 608 (2019).

806. T. Bovornratanaraks , P. Tsuppayakorn-aek, W. Luo and R. Ahuja
Ground–state structure of semiconducting and superconducting phases in xenon carbides at high pressure
Scientific Reports **9,** 2459 (2019).

807. A. Chafai, I. Essaoudi, A. Ainane, F. Dujardin and R. Ahuja
Binding energy of an exciton in a GaN/AlN nanodot: Role of size and external electric field
***Physica B* 559,** 23 (2019).

808. E.Edin, W.Luo, R.Ahuja, B.Kaplan and A.Blomqvist
First principles study of C diffusion in WC/W interfaces observed in WC/Co tools after Ti-alloy machining
***Computational Materials Science* 161,** 236 (2019)

809. M. Behloul, Y. Benhouria, H. Ez-Zahraouy, I. Essaoudi, A. Ainane and R. Ahuja
Theoretical investigation of the electronic and magnetic properties of Zn (Fe, Co) Se: Ab initio calculations and Monte Carlo Simulations
***Superlattices and Microstructures* 127,** 66 (2019).

810. V. Shukla, N. K. Jena, S. R. Naqvi, W. Luo and R. Ahuja
Modeling High-performing Batteries with Mxenes: The case of S-functionalized two-Dimensional Nitride Mxene Electrode
***NanoEnergy* 58,** 877 (2019).

811. S. Umrao, A. K. Maurya, V. Shukla, A. Grigoriev, R. Ahuja, M. Vinayak, R. Srivastava, P. S Saxena, I. Oh and A. Srivastava
Anti-carcinogenic Activity of Blue Fluorescent h-BN Quantum Dots: As an Effective Enhancer for DNA Cleavage Activity of Anti-cancer Drug Doxorubicin
***Materials Today Bio* 1,** 100001 (2019).

812. I.Wani, S.H.M. Jafri, J. Wärnå, A. Hayat, H. Li, V. Shukla, A. Orthaber, A. Grigoriev, R. Ahuja and K. Leifer
Sub 20 nm metal-conjugated molecule junctions acting as a nitrogen dioxide sensor
***Nanoscale* 11,** 6571 (2019).

813. E. Poonia, P. Mishra, V. Poonia, J. Sangwan, R. Kumar, P. Rai, R. Malik, V. K. Tomer, R. Ahuja and Y.K. Mishra,
Aero-gel based CeO2 nanoparticles: Synthesis, structural properties and detailed humidity sensing response
***J. Mat. Chem. C.* 7,** 5477 (2019).

814. E. Anikina, A. Banerjee, V. Beskachko and R. Ahuja,
Importance of Size Effects for Hydrogen Adsorption on Li-functionalized Carbon Nanotubes
***ACS Applied Nano Materials* 2,** 3021 (2019).

815. V. Tomer, R. Malik, V. Chaudhary, Y. Mishra, L. Kienle, R. Ahuja and L. Lin
Superior visible light photocatalysis and low-operating temperature VOCs sensor using cubic Ag(0)-MoS2 loaded g-CN 3D porous hybrid
***Applied Materials Today* 16,** 193 (2019).

816. N. T. Tien, P. T. B. Thao, T-P. Vo and R. Ahuja

Electronic and transport features of sawtooth penta-graphene nanoribbons via substitutional doping
***Physica E* 114,** 113572 (2019).

817. Z. Qian, G. Jiang, Y. Ren, X. Nie and R. Ahuja
Atomistic Modeling of Various Doped Mg2NiH4 as Conversion Electrode Materials for Lithium Storage
***Crystals* 9,** 254 (2019).

818. P. Pakeetood, P. Reunchan, A. Boonchun, S. Limpijumnong, R.Munprom, R. Ahuja, J. T-Thienprasert
Hybrid-Functional Study of Native Defects and W/Mo-Doped in Monoclinic-Bismuth Vanadate
***The Journal of Physical Chemistry C*123,** 14508 (2019).

819. A. Chafai, I. Essaoudi, A. Ainane and R. Ahuja
Linear and nonlinear optical properties of donors inside a CdSe/ZnTe core/shell nanodot: Role of size modulation
***Results in Physics* 14,** 102414 (2019).

820. M. Abdel-Hafiez, R. Thiyagarajan, A. Majumdar, R. Ahuja, W. Luo, A. N. Vasiliev, S.G. Zybtsev, V. Ya. Pokrovskii, S. V. Zaitsev-Zotov, Woei Wu Pai, W. Yang and L.V. Kulik
Pressure-induced reentrant transition in NbS3 phases: Combined Raman scattering and x-ray diffraction study
***Phys. Rev. B.*19,** 235126 (2019).

821. T. Das, S. Chakraborty, R. Ahuja and G.P. Das
Functionalization and Defect Driven Water Splitting Mechanism on Quasi Two-Dimensional TiO_2 Hexagonal Nano sheet
***ACS Applied Energy Materials* 2,** 5074 (2019).

822. T. Watcharatharapong, S. Chakraborty, and R. Ahuja
Mapping Sodium Intercalation Mechanism, Electrochemical Properties and Structural Evolution in Non-stoichiometric Alluaudite $Na_{2+2\delta}Fe_{2-\delta}(SO_4)_3$ Cathode Materials
***Journal of Materials Chemistry A* 7,** 17446 (2019).

823. E. Edin, A. Blomqvist, M. Lattemann, W. Luo & R. Ahuja
MD study of C diffusion in WC/W interfaces observed in cemented carbides
***International Journal of Refractory Metals and Hard Materials* 85,** 105054 (2019).

824. X. Yang, A. Banerjee and R. Ahuja
Probing the Active Sites of Newly Predicted Stable Janus Scandium Dichalcogenides for Photocatalytic Water-splitting
***Catalysis Science & Technology* 9,** 4981 (2019).

825. N. Khossossi, A. Banerjee, Y. Benhouria, I. Essaoudi, A. Ainane and R. Ahuja,
Ab Initio Study of 2D h-BAs monolayer: A promising anode material for Alkali-Metal Ion Batteries

***Physical Chemistry Chemical Physics* 21,** 18328 (2019).

826. A. Das, C. P. Saini, D. Singh, R. Ahuja, A. Kaur, S. Aliukov, D. Shukla and F. Singh
High temperature mediated rocksalt to wurtzite phase transformation in cadmium oxide nano-sheets and their theoretical evidence
***Nanoscale* 11,** 14802 (2019).

827. S. Kansara, S. Gupta, Y. Sonvane, M.V. Pajtler and R. Ahuja,
The Inquisitive Geometric Sites in h-BN Monolayer for Alkali Earth Metal Ion Batteries
***The Journal of Physical Chemistry C* 123,** 19340 (2019).

828. T. Watcharatharapong, S. Chakraborty and R. Ahuja
Defect Thermodynamics in Non-stoichiometric Alluaudite-based Polyanionic Materials for Na-ion Batteries
***ACS Applied Materials & Interfaces* 11,** 32856 (2019).

829. H. Mahida, D. Singh, Y. Sonvane, P. Thakor, R. Ahuja and S. Gupta
The influence of edge structure on the optoelectronic properties of Si2BN quantum dot
***Journal of Applied Physics* 126,** 233104 (2019).

830. C. Ji, L. Bing, W. Liu, J. S. Smith, A. Majumdar, W. Luo, R. Ahuja,
J. Shu, J. Wang, S. Sinogeikin, Y. Meng, V. B. Prakapenka, E. Greenberg, R. Xu, X. Huang,
W. Yang, G. Shen, W. L. Mao and H.K Mao
Ultrahigh pressure isostructural electronic transitions in hydrogen
***Nature* 573,** 558 (2019).

831. X. Nie, Z. Qian, H. Li, R. Ahuja and X. Liu
Theoretical prediction of a novel aluminum nitride nanostructure: Atomistic exposure
***Ceramics International* 45,** 23690 (2019).

832. H. Vovusha, T. Hussain, M. Sajjad, H. Lee, A. Karton, R. Ahuja and U. Schwingenschlögl
Sensitivity Enhancement of Stanene Towards Toxic SO2 and H2S
***Applied Surface Science* 495,** 143622 (2019).

833. J. Prasongkit, V. Shukla, A. Grigoriev, R. Ahuja and V. Amornkitbamrung
Ultrahigh-sensitive gas sensors based on doped phosphorene: A first-principles investigation
***Applied Surface Science* 497,** 143660 (2019).

834. Z. Qian, H. Zhang, G. Jiang, Y. Bai, Y. Ren, W. Du and R. Ahuja
Ab initio Screening of Doped Mg(AlH4)2 Solids for Conversion-type Lithium Storage
***Materials* 12,** 2599 (2019).

835. D.Singh and R.Ahuja
Enhanced optoelectronic and thermoelectric properties by intrinsic structural defects in monolayer HfS2
***ACS Applied Energy Materials* 2,** 6891 (2019).

836. M. B. Johansson, B. Philippe, A. Banerjee, D. Phuyal, S. Mukherjee, S. Chakraborty, M. Cameau, H. Zhu, R. Ahuja, G. Boschloo, H. Rensmo and E. M. J. Johansson
Cesium Bismuth Iodide Solar Cells from Systematic Molar Ratio Variation of CsI and BiI3
***Inorganic Chemistry* 58,** 12040 (2019).

837. A.Banerjee, S. Chakraborty and R. Ahuja,
Rashba Triggered Electronic and Optical Properties Tuning in Mixed Cation-Mixed Halide Hybrid Perovskites
***ACS Applied Energy Materials* 2,** 6990 (2019).

838. X.Yang, D.Singh, Z.Xu, Z.Wang and R.Ahuja,
An emerging Janus MoSeTe material for potential applications in optoelectronic devices
***Journal of Materials Chemistry C* 7,** 12312 (2019).

839. P. Panigrahi, T. Hussain, A. Karton and R. Ahuja,
Elemental Substitution of Two-Dimensional Transition Metal Dichalcogenides (MoSe2 and MoTe2): Implications for Enhanced Gas Sensing
***ACS Sensors* 4,** 2646 (2019).

840. X. Nie, Z. Qian, W. Du, Z. Lu, H. Li, R. Ahuja and X. Liu
Structural evolution of AlN nanoclusters and the elemental adsorption characteristics: Atomistic insight
***NanoMaterials* 9,** 1420 (2019).

841. D. S. Negi, D. Singh, P. A. van Aken and R.Ahuja
Spin-entropy induced thermopower and spin-blockade effect in CoO
***Physical Review B* 100,** 144108 (2019).

842. D. Singh, S. K. Gupta, I. Lukačević, M. Mužević, Y. Sonvane & R. Ahuja
Effect of electric field on optoelectronic properties of indiene monolayer for photoelectric nanodevices
***Scientific Reports* 9,** 17300 (2019).

843. X.Yang, A.Benerjee, Z. Xu, Z. Wang and R.Ahuja
Interfacial aspect of $ZnTe/In_2Te_3$ heterostructures as an efficient catalyst for hydrogen evolution reaction
***Journal of Materials Chemistry A* 7,** 27441 (2019).

844. D.Singh, S. Chakraborty and R. Ahuja,
Emergence of Si_2BN Monolayer as Efficient HER Catalyst under Co-functionalization Influence
***ACS Applied Energy Materials* 2,** 8441 (2019).

845. H. Y. Alniss, Ini-Is. Witzel, M. H. Semreen, P. K. Panda, Y. K. Mishra, R. Ahuja and J. A. Parkinson

Investigation of the Factors That Dictate the Preferred Orientation of Lexitropsins in the Minor Groove of DNA
***Journal of Medicinal Chemistry,* 62,** 10423 (2019).

846. M. Kibbou, Y. Benhouria, M. Boujnah, I. Essaoudi, A. Ainane and R. Ahuja
The electronic, magnetic and electrical properties of Mn2FeReO6: Ab-intio calculations and Monte-Carlo simulation
***Journal of Magnetism and Magnetic Materials* 495,** 165833 (2020).

847. S. S. Deshpande, M. D. Deshpande, T. Hussain and R. Ahuja
Investigating CO2 Storage Properties of C2N Monolayer Functionalized with Small Metal Clusters
***Journal of CO2 Utilization* 35,** 1 (2020).

848. I. Bouziani, Y. Benhouria, I. Essaoudi, A. Ainane and R. Ahuja
High Curie temperature in halfmetallic-ferromagnets (Zn, Cr, Ti)Se and (Zn, Cr, Ti)Te for spintronic devices: Ab initio and Monte Carlo treatments
***Materials Science and Engineering B* 253,** 114484 (2020).

849. I. Bouziani, M. Kibbou, Z. Haman, Y. Benhouria, I. Essaoudi, A. Ainane and R. Ahuja,
Electronic- and optical-properties of ZnO nano-sheet doped and codoped with Be and/or Mg for ultraviolet opto-electronic technologies: density functional calculations
***Physica Scripta* 95,** 015804 (2020).

850. K. Srimathi, T. Hussain, P. Panigrahi, N. G. Subramaniam and R. Ahuja
Influence of Sodium Iodide doped polypyrrole on green synthesized aluminum doped ZnO for the enhanced charge separation at the interface
***Optical Materials* 99,** 109568 (2020).

851. Y. Benhouria, B. Lamarti, A. Oubelkacem, I. Essaoudi, A. Ainane and R. Ahuja
Examination of the Magnetic Properties of the Triangular Type Mixed spin-(1/2, 1) Nanowire
Journal of Superconductivity and Novel Magnetism 33, 817(2020).

852. A. Chafai, I. Essaoudi, A. Ainane and R. Ahuja
Nonlinear optical characteristics of an exciton in a GaSb-capped InSb heterodot: Role of size control
***The European Physical Journal Plus* 135,** 202 (2020).

853. E. Anikina, A. Banerjee, V. Beskachko and R. Ahuja
Li-decorated carbyne for hydrogen storage: charge induced polarization and van't Hoff hydrogen desorption temperature
Sustainable Energy & Fuels 4, 691 (2020).

854. P. Panda, A. Grigoriev, Y.K.Mishra and R. Ahuja
Progress in Supercapacitors: Roles of Two Dimensional Nanotubular Materials
***Nanoscale Advances* 2,** 70 (2020).

855. B. Roondhe, P. K. Jha and R.Ahuja
Haeckelite boron nitride as nano sensor for the detection of hazardous methyl mercury
***Applied Surface Science* 506,** 144860 (2020).

856. P. Panigrahi, A. Kumar, A. Karton, R. Ahuja & T. Hussain,
Remarkable Improvement in Hydrogen Storage Capacities of Two-dimensional Carbon Nitride (g-C3N4) Nanosheets Under Selected Transition Metal Doping
***International Journal of Hydrogen Energy* 45,** 3035 (2020).

857. Z. Nabi, O. Benguerine, B. Bouabdallah, M. Maachou and R. Ahuja,
Structural, elastic, electronic and magnetic properties of Ni2MnSb, Ni2MnSn and Ni2MnSb0.5Sn0.5 magnetic shape memory alloys
Revista Mexicana de Física 66, 121 (2020).

858**.** A. Ahmadivand, B. Gerislioglu, R. Ahuja and Y. K. Mishra
Terahertz Plasmonics: The Rise of Toroidal Metadevices towards Immunobiosensings
Materials Today 32, 108 (2020).

859. H.Tang, X. Gao, J. Zhang, B. Gao, W. Zhou, B.Yan, X. Li, Q. Zhang, S. Peng, D.Huang, L. Zhang, X. Yuan, B. Wan, C. Peng, L. Wu, D. Zhang, H. Liu, L. Gu, F. Gao, T. Irifune, R. Ahuja, H.K.Mao and H. Gou,
Boron-rich Molybdenum Boride with Unusual Short-Range Vacancy Ordering, Anisotropic Hardness, and Superconductivity
Chemistry of Materials 32, 459 (2020).

860. R. Yuksel, O. Buyukcakir, P. K. Panda, S. H. Lee, Y. Jiang, D. Singh, S. Hansen, R. Adelung, Y. K. Mishra, R. Ahuja and R. S. Ruoff
Necklace-like Nitrogen-doped Hollow Carbon 3D Frameworks for Electrochemical Energy Storage
***Advanced Functional Materials* 30,** 1909725 (2020).

861. A. Das, D. Singh, C. Saini, R. Ahuja, A. Kaur and S.Aliukov
Orbital hybridization induced band offset phenomena in NixCd1-xO thin films
Nanoscale 12, 669 (2020).

862. M. Berwanger, R. Ahuja and P. C. Piquini,
HfS2 and TiS2 monolayers with adsorbed C, N, P atoms: a first-principles study
***Catalysts* 10,** 94 (2020).

863. B. Gerislioglu, G. Bakan, R. Ahuja, J. Adam, Y. K. Mishra and A. Ahmadivand
The Role of Ge2Sb2Te5 in Enhancing the Performance of Functional Plasmonic Devices
Materials Today Physics 12, 100178 (2020).

864. S.R.Naqvi, V.Shukla, N.Jena, W.Luo and R.Ahuja
Exploring two-dimensional M2NS2 (M = Ti, V) MXenes based gas sensors for air pollutants
***Applied Materials Today* 19,** 100574 (2020).

865. D. Singh, V. Shukla, P. Panda, Y. Mishra, H-G. Rubahn & R. Ahuja,
Carbon-Phosphide Monolayer with High Carrier Mobility and Perceptible I-V Response for Superior Gas Sensing
***New Journal of Chemistry* 44,** 3777 (2020).

866. S.R.Naqvi, T.Hussain, S.R.Gollu, W.Luo and R.Ahuja
Superior Sensitivity of Metal Functionalized Boron Carbide (BC3) Monolayer Towards Carbonaceous Pollutants
***Applied Surface Science* 512,** 145637 (2020).

867. P. Mishra, D. Singh, Y. Sonvane and R. Ahuja
2D monolayer boron sulfide as an efficient material for optical nanodevices
***AIP Conference Proceedings* 2220,** 130039 (2020).

868. S. Gahlot, F. Dappozze, D. Singh, R. Ahuja, L. Cardenas, L. Burel, D. Amans, C. Guillard, Chantal & S. Mishra
Room-temperature conversion of Cu2-xSe to CuAgSe nanoparticles to enhance photocatalytic performance of its composites with TiO2
Dalton Transactions 49, 3580 (2020).

869. V.Shukla, A. Grigoriev and R. Ahuja
Rectifying behavior in twisted bilayer black phosphorus nanojunction mediated through intrinsic anisotropy
Nanoscale Advances 2, 1493 (2020).

870. I. Bouziani, Z. Haman, M. Kibbou, Y. Benhouria, I. Essaoudi, A. Ainane and R. Ahuja,
Electronic- and optical-properties of penta-SiC2 and -SiGeC4 monolayers for solar energy conversion
***Superlattices and Microstructures* 142,** 106524 (2020).

871. D. Singh, P. Panda, Y. Mishra & R. Ahuja,
Van der Waals induced molecular recognition of canonical DNA nucleobases on 2D GaS monolayer
Physical Chemistry Chemical Physics 22, 6706 (2020).

872. X. Zhao, X. Yang, D. Singh, P. Panda, W. Luo, Y. Li & R. Ahuja
Strain Engineered Metal Free h- B2O Monolayer as a Mechanocatalyst for Photocatalysis and Improved Hydrogen Evolution Reaction
***The Journal of Physical Chemistry C* 124,** 7884 (2020).

873. P. Mishra, D. Singh, Y. Sonvane & R. Ahuja
Enhancement of hydrogen storage capacity on co-functionalized GaS monolayer under external electric field
***International Journal of Hydrogen Energy* 45,** 12384 (2020).

874.T. Hussain, M. Sajjad, D. Singh, H. Bae, H. Lee, J. A. Larsson, R. Ahuja and A. Karton
Sensing of Volatile Organic Compounds on Two-Dimensional Nitrogenated Holey Graphene, Graphdiyne, and Their Heterostructure
***Carbon* 163,** 213 (2020).

875. M. Zidane, El M. Salmani, A. Majumdar, H. Ez-Zahraouy, A. Benyoussef and R. Ahuja
Electrical and Thermal Transport Properties of Fe–Ni Based Ternary Alloys in the Earth's Inner Core: An ab initio Study
***Physics of the Earth and Planetary Interiors* 301,** 106465 (2020).

876. A. Allal, M Halit, S. Saib, L. Azzouz, S. Maabed, M. Bouchenafa and R. Ahuja,
A Comparative theoretical investigation of optoelectronic and mechanical properties of KYS2 and KLaS2
Materials Science in Semiconductor Processing 113, 105048 (2020).

877. H. R. Mahida, D. Singh, P. K. Panda, Y. Sonvane, P. B. Thakor and R. Ahuja
Electronic and optical properties of a structural defect in 2D MgF_2 monolayer
***AIP Conference Proceedings* 2220,** 100008 (2020).

878. X.Yang, W.Luo and R.Ahuja
Fluoride ion batteries: Designing flexible M2CH2 (M=Ti or V) MXenes as high-capacity cathode materials
***Nano Energy* 74,** 104911 (2020).

879. P. Mishra, D. Singh, Y. Sonvane & R. Ahuja
Two-Dimensional Boron Monochalcogenide Monolayer for Thermoelectric Material
***Sustainable Energy & Fuels* 4,** 2363 (2020).

880. Z. Liu, R. Ahuja, H. Li, and W. Luo
Mechanical and electronic properties of van der Waals layered hcp PdH2
***Scientific Reports* 10,** 8037 (2020).

881. C. Ji, B. Li, W. Liu, J. Smith, A. Bjorling, A. Majumdar, W. Luo, R. Ahuja, J. Shu, J. Wang, S. Sinogeikin, Y. Meng, V. Prakapenka, E. Greenberg, R. Xu, X-R. Huang, Y. Ding, A. Soldatov, W. Yang, G. Shen, W. Mao and H-k Mao
Crystallography of Low Z material at Ultrahigh Pressure: Case Study on Solid Hydrogen
***Matter and Radiation at Extremes* 5,** 038401 (2020).

882. A. Majumdar, X. Yang, W. Luo, S. Chowdhury, S. Chakraborty and R. Ahuja,
High exothermic dissociation in van der Waals like hexagonal two dimensional nitrogene from first-principles molecular dynamics
***Applied Surface Science* 529,** 146552 (2020).

883. X.Yang, D.Singh, Z.Xu and R.Ahuja
Sensing the polar molecules MH_3 (M=N, P, or As) with Janus NbTeSe monolayer
***New Journal of Chemistry* 44,** 7932 (2020).

884. X. Zhao, P. Panda, D. Singh, X. Yang; Y. K. Mishra and R. Ahuja
2D g-C3N4 monolayer for amino acids sequencing
***Applied Surface Science* 528,** 146609 (2020).

885. P. Mishra, D. Singh, Y. Sonvane & R. Ahuja
Metal-functionalized 2D boron sulfide monolayer material enhancing hydrogen storage capacities
***Journal of Applied Physics* 127,** 184305 (2020).

886. D. Singh, P. Panda, N. Khossossi, Y. K. Mishra, A. Ainane, R. Ahuja
Impact of edge on interfacial interactions and efficient visible-light photocatalytic activity of metal-semiconductor hybrid 2D materials
***Catalysis Science & Technology* 10,** 3279 (2020).

887. E. Anikina, A. Banerjee, V. Beskachko and R. Ahuja
Influence of Kubas-type Interaction of B-Ni Codoped Graphdiyne with Hydrogen Molecules on Desorption Temperature and Storage Efficiency
***Materials Today Energy* 16,** 100421 (2020).

888. A.Nair, R.Ahuja and B.Pathak
Unravelling Single Atom Electrocatalytic Activity of Transition Metal Doped Phosphorene
Nanoscale Advances 2, 2410 (2020).

889. N. T. Tien, P. T. B. Thao, P. V. Trung and R. Ahuja
Influence of edge termination on the electronic and transport properties of sawtooth penta-graphene nanoribbons
***Journal of Physics and Chemistry of Solids* 146,** 109528 (2020).

890. S. Gahlot, E. Jeanneau, D. Singh, P.K. Panda, Y.Mishra, R. Ahuja, G. Ledoux & S. Mishra,
Molecules Vs nanoparticles: Identifying a reactive molecular intermediate in the synthesis of ternary coinage metal chalcogenides
***Inorganic Chemistry* 59,** 7727 (2020).

891. N. Khossossi, V. Shukla, Y. Benhouria, I. Essaoudi, A. Ainane, R. Ahuja, G. Babu and P. M. Ajayan
Exploring the Possibility of β-phase Arsenic-Phosphorus Polymorph Monolayer as Anode Materials for Sodium-ion Batteries
Advanced Theory and Simulations 3, 2000023(2020).

892. W. Du, C. Zhao, K. Liu, H. Li, Y. Chen, Y. Bai, R. Ahuja & Z. Qian
Defective and Doped Aluminum Nitride Monolayers for 2 NO Adsorption: Physical Insight
Chemical Physics Letters 753, 137592 (2020).

893. P. K. Panda, M. N. Arul, P. Patel, S. K. Verma, W. Luo, H-G. Rubahn, Y. K. Mishra, M. Suar and R. Ahuja,
Structure-based drug designing and immunoinformatics approach for 2019-nCoV

Science Advances 6, eabb8097 (2020).

894. P. Panigrahi, A. Kumar, H. Bae, H. Lee, R. Ahuja and T. Hussain
Capacity Enhancement of Polylithiated Functionalized Boron Nitride Nanotubes: An Efficient Hydrogen Storage Medium
***Physical Chemistry Chemical Physics* 22,** 15675 (2020).

895. H. Wang, R. Emanuelsson, A. Banerjee, R. Ahuja, M. Strømme and M. Sjödin,
Effect of Cycling Ion and Solvent on the Redox Chemistry of Substituted Quinones and Solvent-Induced Breakdown of the Correlation Between Redox Potential and Electron Withdrawing Power of Substituents
The Journal of Physical Chemistry C 124, 13609 (2020).

896. K. Kotmool, P.Tsuppayakorn-aek, T.Kaewmaraya, U.Pinsook, R.Ahuja, T. Bovornratanaraks
Structural Phase Transitions, Electronic Properties and Hardness of RuB4 under High Pressure in Comparison with FeB4 and OsB4
The Journal of Physical Chemistry C 124, 14804 (2020).

897. A.Benerjee, S. Chakraborty and R. Ahuja
Reaction Coordinate Mapping of Hydrogen Evolution Mechanism on Mg3N2 Monolayer
International Journal of Hydrogen Energy 45, 22848 (2020).

898. Y. Benhouria, M. Kibbou, N. Khossossi, J. Foshi, I. Essaoudi, A. Oubelkacem, A. Ainane and R. Ahuja
Carbides-anti-perovskites Mn3(Sn, Zn)C : Potential candidates for an application in magnetic refrigeration
***Physica E* 124,** 114317 (2020).

899. N. Khossossi, Y. Benhouria, S.R.Nqvi, P.K.Panda, I. Essaoudi, A. Ainane and R. Ahuja
Hydrogen storage characteristics of Li and Na decorated 2D Boron Phosphide
Sustainable Energy & Fuels 4, 4538 (2020).

900. H. Zhang, W. Du, T. Zhao, R. Ahuja and Z. Qian
Poisonous vapor adsorption on pure and modified aluminum nitride nanosheet for environmental safety: A DFT exploration
Sustainability 12, 10097(2020).

901. A. Patel, D. Singh, Y. Sonvane, P.B. Thakor and R. Ahuja
Bulk and monolayer As2S3 as promising thermoelectric material with high conversion performance
Computational Materials Science 183, 109913 (2020).

902. A. Majumdar, S. Chakraborty and R. Ahuja
Emerging Piezochromism in Transparent Lead free Perovskite Rb3X2I9 (X = Sb, Bi) under Compression: A Comparative Theoretical Insight
Journal of Applied Physics 128, 045102 (2020).

903. N. Khossossi, P.K.Panda, D. Singh, V. Shukla, Y.Mishra, I. Essaoudi, A. Ainane and R.Ahuja,
Rational Design of 2D h-BAs Monolayer as Advanced Sulfur hosts for High Energy Density Li-S Batteries
ACS Applied Energy Materials 3, 7306 (2020).

904. E. Anikina, T. Hussain, V. Beskachko, H. Bae, H. Lee and R. Ahuja,
Tunning Hydrogen Storage Properties of Carbon Ene-Yne (CEY) Nanosheets through Selected Foreign Metal Functionalization
The Journal of Physical Chemistry C 124, 16827 (2020).

905. A. Allal, M. Bouchenafa, M. Halit, S. Saib, Z. Liu, W. Luo and R. Ahuja
Structural stability, mechanical, electronic and optical behaviour of RbXS2 (X = Y and La) under high pressure: A first-principle study
Journal of Alloys and Compounds 848, 156401 (2020).

906. X.Yang, A.Banerjee and R.Ahuja
Structural Insight of the Frailty of 2D Janus NbSeTe as an Active Photocatalyst
ChemCatChem 12, 6013 (2020).

907. P. Tsuppayakorn-aek, U. Pinsook, W. Luo, R. Ahuja and T. Bovornratanaraks,
Superconductivity of Superhydride CeH10 under High Pressure
Materials Research Express *7* 086001 (2020).

908. E. Anikina, T. Hussain, V. Beskachko and R. Ahuja,
Elucidating Hydrogen Storage Properties of Two-Dimensional Siligraphene (SiC8) Monolayers Upon Selected Metal Decoration
Sustainable Energy & Fuels 4, 5578 (2020).

909. D. Singh, V. Shukla and R.Ahuja,
Optical excitations and thermoelectric properties of two-dimensional holey graphene
Physical Review B 102, 075444 (2020).

910. A. Majumdar, D. VanGennep, J. Brisbois, D. Chareev, A. V. Sadakov, A. S. Usoltsev, M. Mito, A.V. Silhanek, T. Sarkar, A. Hassan, O. Karis, R. Ahuja and M. Abdel-Hafiez
Interplay of charge density wave and multiband superconductivity in layered quasi two-dimensional: The case of 2H-NbS2 and 2H-NbSe2
Physical Review Materials 4, 084005 (2020).

911. B. Roondhe, V. Sharma, H. L. Kagdada, D. K. Singh, T. Saha Dasgupta and R. Ahuja
Enhancing the electronic and phonon transport properties of two-dimensional hexagonal boron nitride through oxygenation: A first principles study
Applied Surface Science 533, 147513(2020).

912. R. Kumar, K. Mondal, P.K.Panda, A.Kaushik, R. Abolhassani, R.Ahuja, H-G. Rubahn, Y. K.Mishra
Core-Shell Nanostructures: Perspectives towards Drug Delivery Applications
Journal of Materials Chemistry B 8, 8992 (2020).

913. P. Bhuyan, Y. Sonvane, P. Gajjar, R. Ahuja and S. Gupta,
Ultrathin nanowire PdX_2 (X= P, As): stability, electronic transport and thermoelectric properties
New Journal of Chemistry 44, 15617 (2020).

914. N. Khossossi, D. Singh, A. Ainane and R. Ahuja
Recent progress of defect chemistry on 2D materials for advanced battery anodes
Chemistry - An Asian Journal 15, 3390 (2020).

915. P. Panigrahi, S.B. Mishra, T. Hussain, B. Nanda and R. Ahuja
Density Functional Theory Studies of Si2BN Nanosheets as Anode Materials for Magnesium Ion Batteries
ACS Applied Nano Materials 3, 9055 (2020).

916. A. Ahmadivand, B. Gerislioglu, R. Ahuja and Y. K. Mishra
Toroidal Metaphotonics and Metadevices
Laser & Photonics Reviews 14, 1900326 (2020).

917. A. Majumdar, S. Chowdhury and R. Ahuja,
Ultralow Thermal Conductivity and High Thermoelectric Figure of Merit in Two Dimensional Thallium Selenide
ACS Applied Energy Materials 3, 9315 (2020).

918. A. Das, D. Singh, A. Kaur, C. Saini, D. Kanjilal, C. Balasubramanian, J. Ghosh and R. Ahuja
Temperature dependent cationic doping driven phonon dynamics investigation in CdO thin films using Raman Spectroscopy
The Journal of Physical Chemistry C 124, 21818 (2020).

919. Y. Ren, X. Ren, R. Ahuja and Z. Qian
First-principles calculations into $LiAl(NH_2)_4$ and its derivative hydrides for potential sodium storage
Results in Physics* 19,** 103408(2020)***

920. A. Patel, D. Singh, Y. Sonvane, P.B. Thakor and R. Ahuja
High thermoelectric performance in two dimensional Janus monolayer material WS-X (X=Se, Te)
ACS Applied Materials & Interfaces 12, 46212 (2020).

921. X. Zhao, X. Yang, Y.Li and R. Ahuja
Exploring the Degradation Behavior of Ce-Monazite in Water Solution Through Adsorption and Penetration Kinetics
The Journal of Physical Chemistry C 124, 22173(2020).

922. P. Sharma, M. Minakshi Sundaram, T. Watcharatharapong, D. Laird, H. Euchner and R. Ahuja
Zn metal atom doping on the surface plane of 1D NiMoO4 nanorods with improved redox chemistry
ACS Applied Materials & Interfaces 12, 44815 (2020).

923. X. Yang, D. Singh and R. Ahuja
Recent advancements and future prospects in 2D semiconductor-based photocatalysts for water splitting
Catalysts **10,** 1111 (2020).

924. P. Mishra, D. Singh, Y. Sonvane and R. Ahuja
Excitonic effects in the optoelectronic properties of graphene-like BC monolayer
Optical Materials **110,** 110476 (2020).

925. P. Tsuppayakorn-aek, X. Yang, P. Pluengphon W. Luo, R. Ahuja and T. Bovornratanaraks
Route to high Tc superconductivity of BC7 via strong bonding of boron-carbon compound at high pressure
Scientific Reports 10, 18090 (2020).

926. Q. Liang, X. Nie, W. Du, P. Zhang, J. Ping, R. Ahuja, J. Ping and Z. Qian
First-principles exploration of hazardous gas molecules adsorption on pure and modified Al60N60 nanoclusters
Nanomaterials. 10, 2156 (2020).

927. Z. Haman, M. Kibbou, I. Bouziani, Y. Benhouria, I. Essaoudi, A. Ainane and R. Ahuja
Structural, Electronic and optical properties of two-dimensional Janus transition metal oxides MXO (M=Ti, Hf and Zr; X=S and Se) for photovoltaic and opto-electronic applications
Physica B: Physics of Condensed Matter. 604, 412621(2020).

928. P. Panigrahi, K. Alhameedi, A. Karton, R. Ahuja and T.Hussain
Improved Adsorption and Migration of Divalent Ions Over C4N Nanosheets: Potential Anode for Divalent Batteries
Surfaces and Interfaces 21, 100758 (2020).

929. P. Sharma, M. Minakshi Sundaram, D. Singh and R. Ahuja
A Highly Energetic and Stable Gadolinium/Bismuth Molybdate with a Fast Reactive Species, Redox Mechanism of Aqueous Electrolyte
ACS Applied Energy Materials 3, 12385 (2020).

930. A. Majumdar, A. Adeleke, S. Chakraborty and R. Ahuja
Emerging Piezochromism in Lead free Alkaline Earth Chalcogenide Perovskite AZrS3 (X = Mg, Ca, Sr and Ba) under Pressure
Journal of Materials Chemistry C 8, 16392 (2020).

931. D. Singh, V. Shukla, N. Khossossi, A. Ainane and R. Ahuja,

Harnessing the unique properties of MXenes for advanced rechargeable batteries
Journal of Physics: Energy 3, 012005 (2020).

932. D. Singh, M. Sajjad, J. A. Larsson and R. Ahuja
Promising high-temperature thermoelectric response of bismuth oxybromide
Results in Physics 19, 103584 (2020).

933. T. R. Arslanov, U. Z. Zalibekov, L. Kilanski, I. V. Fedorchenko, T. Chatterji and R. Ahuja
Large pressure-induced magnetoresistance in a hybrid ferromagnet-semiconductor system: Effect of matrix modification on the spin-dependent scattering
Journal of Applied Physics 128, 213903 (2020).

934. D.Singh and R.Ahuja
Highly sensitive gas sensing material for environmentally toxic gases based on Janus NbSeTe monolayer
Nanomaterials 10, 2554 (2020).

935. M. Kibbou, Z. Haman, I. Bouziani, N. Khossossi, Y. Benhouria, I. Essaoudi, A. Ainane and R. Ahuja
Cs2InGaX6 (X=Cl, Br, or I): Emergent Inorganic Halide Double Perovskites with enhanced optoelectronic characteristics
Current Applied Physics 21, 50 (2021).

936. D. Raval, B. Babariya, S.K. Gupta, R. Ahuja and P.N. Gajjar
Ultrahigh carrier mobility and light harvesting performance of 2D penta-PdX2 monolayer
Journal of Materials Science 56, 3846 (2021).

937. T. Kaewmaraya, L. Ngamwongwan, P. Moontragoon, W. Jarernboon, D. Singh, R. Ahuja, A. Karton and T. Hussain
Novel Green Phosphorene as a Superior Chemical Gas Sensing Material
Journal of Hazardous Materials 401, 123340 (2021).

938. P. Panigrahi, D. Jini, H. Bae, H. Lee, R. Ahuja and T.Hussain
Two-Dimensional Janus Monolayers of MoSSe as Promising Sensor Towards Selected Adulterants Compounds
Applied Surface Science 542, 148590 (2021).

939. N. Khossossi, A. Banerjee, I. Essaoudi, A. Ainane, P. Jena and R. Ahuja
Thermodynamics and kinetics of 2D g-GeC monolayer as an anode materials for Li/Na-ion batteries
Journal of Power Sources 485, 229318 (2021).

940. X.Yang, T. Hussain, J.Wårnä, Z.Xu and R.Ahuja
Exploring Janus MoSSe monolayer as a workable media for SOF6 decompositions sensing based on DFT calculations
Computational Materials Science 186, 109976(2021).

941. P. D. Bhuyan, S. K. Gupta, P. N. Gajjar, and R. Ahuja
Metallic one-dimensional heterostructure for gas molecule sensing
Scientific Reports 11, 433 (2021).

942. S. Wang, X. Zhao, X. Wu, Q. Zhang, Y. Teng, R. Ahuja and Y. Zhang
Design of continuous transport of droplet by contact-boiling regime
Langmuir 37, 553 (2021).

943. P. Tsuppayakorn-aek, P. Phansuke, P. Kaewtubtim, R. Ahuja, and T. Bovornratanaraks
Enthalpy stabilization of superconductivity in an alloying S-P-H system: First-principles cluster expansion study under high pressure
***Computational Materials Science* 190,** 110282 (2021).

944. D. Singh, S. K. Gupta, N. Seriani, I. Lukačević, Y. Sonvane, P. N. Gajjar and R. Ahuja
Mechanism of formaldehyde and formic acid formation on (101)-TiO2@Cu4 system through CO2 hydrogenation
***Sustainable Energy & Fuels* 5,** 564 (2021).

945. P. Panigrahi, M. Desai, M. K. Talari, H. Bae, H. Lee, R. Ahuja and T.Hussain
Selective Decoration of Nitrogenated Holey Graphene (C2N) with Titanium Clusters for Enhanced Hydrogen Storage Application
***International Journal of Hydrogen Energy* 46,** 7371 (2021).

946. P. Pluengphon, P. Tsuppayakorn-aek, B. Inceesungvorn, R. Ahuja and T. Bovornratanaraks
Formation of lightweight ternary polyhydride and hydrogen storage mechanism
The Journal of Physical Chemistry C. 125, 3, 1723(2021).

947. T.Y.Mi, N.D.Khanh, R.Ahuja and N.T.Tien
Diverse structural and electronic properties of pentagonal SiC2 nanoribbons: A first-principles study
Materials Today Communications 26, 102047 (2021).

948.E. Edin, A. Blomqvist, W. Luo and R. Ahuja
Large scale screening of interface parameters in the WC/W system using classical force field and first principles calculations
The Journal of Physical Chemistry C 125, 3631 (2021).

949. S. Wang, X. Zhao, Y. Teng, X. Chen and R. Ahuja
Large-scale fabrication of wettability-controllable coatings for optimizing condensates transfer ability
Langmuir 37, 2476 (2021).

950. V.Shukla, R. Kumawat, N. Jena, B.Pathak and R. Ahuja
Electronic and Transport Properties of Bilayer Phosphorene Nanojunction: Effect of Paired Substitution Doping

ACS Applied Electronic Materials 3, 733 (2021).

951. P. Tsuppayakorn-aek, W. Sukmas, R.Ahuja, W. Luo and T. Bovornratanaraks
Stabilization and electronic topological transition of hydrogen–rich metal Li_5MoH11under high pressures from First-principles predictions
Scientific Reports 11, 4079 (2021).

952. A. Bandyopadhyay, A. Majumdar, S. Chowdhury, R. Ahuja and D. Jana
8-16-4 graphyne: Square lattice two-dimensional nodal line semimetal with non-trivial topological Zak index
Phys. Rev. B. 103, 075137 (2021).

953. J. Tang, Y. Teng, Y. Chen, X. Zhao, S. Wang, W.Wang and R. Ahuja
Reduction of the sintering temperature and dielectric loss of the CCTO ceramic by doping tellurite glass
Ceramics International 47, 10006 (2021).

954. M.C. Sahu, S.K- Mallik, S.Sahoo, S.Gupta, R.Ahuja and S.P. Sahoo,
Effect of Charge Injection on the Conducting Filament of Valence Change Anatase TiO2 Resistive Random Access Memory Device
***The Journal of Physical Chemistry Letters* 12,** 1876 (2021).

955. S.K.Verma, E. Jha, P. K Panda, P. Patel, P. Kumari, S. Bhaumik, S.K.S. Parashar, R. Ahuja and M. Suar
Intrinsic atomic interaction at molecular proximal vicinity infer cellular biocompatibility of antibacterial nano-pepper
Nanomedicine 16, 307 (2021).

956. H.Mahida, D.Singh, Y. Sonvane, S. Gupta, P. Thakor and R. Ahuja,
Hydrogenation and oxidation enhanced the thermoelectric performance of Si_2BN monolayer
New Journal of Chemistry 45, 3892 (2021).

957. D. Singh, N. Khossossi, A. Ainane and R. Ahuja
Modulation of 2D GaS/BTe vdW heterostructure as an efficient HER Catalyst under external electric field influence
Catalysis Today 370, 14 (2021).

958. P Tsuppayakorn-aek, J Zhang, W Luo, Y Ding, R Ahuja and T. Bovornratanaraks
Bain Deformation Mechanism and Lifshitz Transition in Magnesium under High Pressure
physica status solidi (b) 258, 2000279 (2021).

959. T. Das, S.Chakraborty, R. Ahuja, Y. Kawazoe and G. P Das
Charge Transfer Driven Interaction of CH4, CO2 and NH3 with TiS2 Monolayer: Influence of Vacancy Defect
Catalysis Today. 370, 189 (2021).

960. R. Tian, S. Zhao, J. Li, Z. Chen, W. Peng, Y. He, L. Zhang, S. Yan, L. Wu, R. Ahuja and H. Gou
Pressure-Promoted Highly-Ordered Fe-doped-Ni_2B for Effective Oxygen Evolution Reaction and Overall Water Splitting
Journal of Materials Chemistry A 9, 6469 (2021).

961. G.L.Cardoso, P.Piquini and R.Ahuja
From monolayers to nanotubes: towards catalytic transition metal dichalcogenides for hydrogen evolution reaction
Energy & Fuels.35, 6282 (2021).

962. M. Boota, T. Hussain, L. Yang, M. Bécuwe, W. Porzio, L. Barba and R. Ahuja
Mechanistic understanding of the interactions and pseudocapacitance of multi-electron redox organic molecules sandwiched between MXene layers
Advanced Electronic Materials 7, 2001202 (2021).

963. Z. Haman, N. Khossossi, M. Kibbou, I. Bouziani, D. Singh, I. Essaoudi, A. Ainane and R. Ahuja
Computational identification of efficient 2D Aluminium chalcogenides monolayers for optoelectronics and photocatalysts applications
Applied Surface Science.556, 149561 (2021).

964. S. Verma, P. Panda, P. Kumari, P. Patel, A. Arunima, E. Jha, S. Husain, R. Prakash, R. Hergenröder, Y. Mishra, R. Ahuja, R. Varma and M. Suar,
Determining factors for the nano-biocompatibility of cobalt oxide nanoflakes: Proximal discrepancy in intrinsic atomic interaction at differential vicinage
Green Chemistry 23, 3439 (2021).

965. S. Mallik, S. Sahoo, M. Sahu, S. Gupta, S. Dash, R. Ahuja and S. Sahoo
Salt-assisted Growth of Monolayer MoS2 for High Performance Hysteresis Free Field Effect Transistor
J. Applied Physics 129, 145106 (2021).

966. B. Roondhe, S. P. Sanyal, P. K. Jha, R. Ahuja, S. Shukla and S. Saxena
H- and T- Li2O monolayers: Latest addition to 2D Flatlands
Applied Surface Science 556, 149737 (2021).

967. . P. Panigrahi, Y. Pal, T. Hussain and R. Ahuja
Application of Germanene Monolayers as Efficient Anchoring Material to Immobilize Lithium Polysulphides in Li-S Batteries
Applied Surface Science 558, 149850 (2021).

968. M. K. Aslam, Y. Niu, T. Hussain, H. Tabassum, W. Tang, M. Xu and R. Ahuja
How to avoid dendrite formation in metal batteries: Innovative strategies for dendrite suppression
***Nano Energy* 86,** 106142 (2021).

969. S. Deshpande, M. Deshpande, K. Alhameedi, R. Ahuja and T. Hussain
Carbon Nitride Monolayers as Efficient immobilizers Towards Lithium Selenides : Potential Applications in Lithium-Selenium Batteries
ACS Applied Energy Materials 4, 3891 (2021).

970. B. R. Sahoo; P. K. Panda; W. Liang; W.-J. Tang; R. Ahuja and A. Ramamoorthy,
Degradation of Alzheimer's amyloid-β by a catalytically inactive insulin-degrading enzyme,
Journal of Molecular Biology 433, 166993 (2021).

971. P. Panigrahi, D. Acharya; S. R. Selvi, R. Ahuja and T.Hussain
Enhancing Energy Storage Efficiency of Lithiated Carbon Nitride (C7N6) Monolayers Under Co-Adsorption of H2 and CH4
International Journal of Hydrogen Energy 46, 19988 (2021).

972. D. Singh, S. Gupta, T. Hussain, Y. Sonvane, P. N. Gajjar and R. Ahuja
Antimonene Allotropes α- and β-Phases as Promising Anchoring Material for Lithium-Sulfur Batteries
Energy & Fuels 35, 9001 (2021).

973. G.L.Cardoso, P.Piquini, N. Khossossi and R.Ahuja
Lithium-Functionalized Boron Phosphide Nanotubes (BPNTs) as an efficient Hydrogen Storage carrier
International Journal of Hydrogen Energy 46, 20586 (2021).

974. A. Majumdar, S. Chowdhury and R. Ahuja
Drastic Reduction of Thermal Conductivity in Hexagonal AX (A= Ga, In & Tl, X = S, Se & Te) Monolayers due to Alternative Atomic Configuration
Nano Energy 88, 106248 (2021).

975 P. Tsuppayakorn-Aek, N. Phaisangittisakul, R. Ahuja & T. Bovornratanaraks
High-temperature superconductor of sodalite-like clathrate hafnium hexahydride
Scientific Reports 11, 16403 (2021).

976. R. Somaiya, D.Singh, Y. Sonvane, S. Gupta and R. Ahuja,
Potential SiX (X = N, P, As, Sb, Bi) homo-bilayers for visible-light photocatalysts application
Catalysis Science & Technology 11, 4996 (2021).

977. P. Panigrahi, Y. Pal, R. Ahuja, and T. Hussain,
Exploring the full potential of functional Si_2BN nanoribbons as highly reversible anode materials for Mg-ion battery
Energy & Fuels 35, 12688 (2021).

978. G. Damas, L. Costa, R. Ahuja, and M. Araujo
Understanding Carbon Dioxide Capture on Metal-Organic Frameworks from First-Principles Theory: The Case of MIL-53(X), with X= Fe,$^{3+}$ Al^{3+} and Cu^{2+}
The Journal of Chemical Physics 155, 024701 (2021).

979. Z. Haman, N. Khossossi, M. Kibbou, I. Bouziani, I. Essaoudi, A. Ainane and R. Ahuja
Two-dimensional Janus Sn2SSe and SnGaS2 semiconductors as strong absorber candidates for photovoltaic solar cells: First principles computations
Physica E 134, 114900 (2021).

980. D. Negi, D. Singh, R. Ahuja & P. A. van Aken
Coexisting commensurate and incommensurate charge ordered phases in CoO
Scientific Reports 11, 19415 (2021).

981. I Bouziani, Z Haman, M Kibbou, I Essaoudi, A Ainane and R Ahuja
Electronic, optical and thermoelectric properties of two-dimensional pentagonal SiGeC4 nanosheet for photovoltaic applications: First-principles calculations
Superlattices and Microstructures **158,** 107024 (2021).

982. J. Sun, P. K. Panda, S. Samal, R. Ahuja, S. Ajeganova, I. Hafström, A. Liu and J. Frostegård
Effects of atorvastatin on T cell activation and apoptosis in systemic lupus erythematosus and novel simulated interactions with CRP and IL-6
ACR Open Rheumatology 3, 642 (2021).

983. X. Yang, J. Wärnå, J. Wang, P. Zhang, W. Luo and R. Ahuja
Enhanced overall water splitting under visible light of MoSSe| WSSe heterojunction by lateral interfacial engineering
Journal of Catalysis **404,** 18 (2021).

984. S. K Verma, A. Thirumurugan, P. K. Panda, P. Patel, A. Nandi, E. Jha, K. Prabakaran, R. Udayabhaskar, R.V. Mangalaraja, Y. K. Mishra, A. A-Fakhrabadi, M. J. Morel, M. Suar and R. Ahuja
Altered electrochemical properties of Iron oxide nanoparticles by carbon enhance molecular biocompatibility through discrepant atomic interaction
Materials Today Bio **12,** 100131 (2021).

985. H. Zhang, W. Du, J. Zhang, R. Ahuja & Z. Qian
Nitrogen-Containing Gas Sensing Properties of 2-D Ti2N and Its Derivative Nanosheets: Electronic Structures Insight
Nanomaterials **11,** 2459 (2021).

986. A. R. Patel, D. Singh, Y. Sonvane, P.S. Thakor and R. Ahuja
Impact of stacking on the optoelectronic properties of 2D ZrS2/GaS heterostructure
Materials Today: Proceedings **47,** 526 (2021).

987. C. Murugesan, S. P. Panjalingam, S. Lochab, R. K. Rai, X. Zhao, D. Singh, R. Ahuja & P. Barpanda
Cobalt tetraphosphate as an efficient bifunctional electrocatalyst for hybrid sodium-air batteries
Nano Energy 89, 106485 (2021).

988. M. Boota, E. Jung, R. Ahuja and T. Hussain,
MXene binder stabilizes pseudocapacitance of conducting polymers
***Journal of Materials Chemistry A* 9,** 20356 (2021).

989 D. Gupta, S. Chakraborty, R. Amorim, R. Ahuja and T. Nagaiah,
Local electrocatalytic activity of PtRu supported on nitrogen doped carbon nanotubes towards methanol oxidation by scanning electrochemical microscopy
***Journal of Materials Chemistry A* 9,** 21291 (2021).

990. A.S.Nair, A.Anoop, R.Ahuja and B.Pathak
Role of atomicity in the oxygen reduction reaction activity of platinum sub nanometer clusters: A global optimization study
***Journal of Computational Chemistry* 42,** 1944 (2021).

991. H.R. Mahida, D. Singh, Y. Sonvane, R. Ahuja and P.B. Thakor
2D MgF2 nanosheet as a promising candidate for thermoelectric material
***Materials Today: Proceedings* 47,** 555 (2021).

992. S. K. Verma, A. Nandi, A. Sinha, P. Patel, E. Jha, S. Mohanty, P. K. Panda, R. Ahuja, Y. K. Mishra, M. Suar
Zebrafish (Danio rerio) as an ecotoxicological model for Nanomaterial induced toxicity profiling
***Precision Nanomedicine* 4,** 750 (2021).

993. P. Tsuppayakorn-aek, A. Ektarawong, P. Jimlim, N. Kanchanavatee, R. Ahuja, W. Luo and T. Bovornratanaraks
Structural predictions of superconducting phase in tungsten ditellurides WTe2 from first-principles evolutionary techniques under high pressure
***Computational Materials Science* 200,** 110795 (2021).

994. K. Lakhani, S. Kansara, S. K Gupta, Y. Sonvane, D. Seifu, P.N. Gajjar & R. Ahuja
Dissociation of air pollutant on the uniform surface of pentagonal BeP2
Applied Surface Science 570, 151061 (2021).

995. S.Sahoo, M.C. Sahu, S.K. Mallik, N. Sharma, A.K. Jena, S. Gupta, R.Ahuja and S Sahoo,
Electric field Modulated Charge transfer in Geometrically Tailored MoX2/WX2 (X=S, Se) Heterostructures
***The Journal of Physical Chemistry C* 125,** 22360 (2021).

996. T. Bovornratanaraks, R. Ahuja and P. Tsuppayakorn-aek
Semiconducting phase of hafnium dioxide under high pressure: a theoretical studied by quasi-particle GW calculations
Materials Research Express 8, 105901 (2021).

997. A. Kaur, D. Singh, A. Das, S. Singh, K. Asokan, L. Singh, I. B Mishra and R. Ahuja
Correlation between Reduced Dielectric Loss and Charge Migration Kinetics in NdFeO3 Modified Ba0.7Sr0.3TiO3 Ceramics

J Mater Sci: Mater Electronics 32, 24910 (2021).
998. S. G-Parra, Ó. Gomis, R. Vilaplana, V. P. C-Gotor, D. M-García, P. R-Hernández, A. Muñoz, A. Romero, A. Majumdar, R. Ahuja, C. Popescui and F. J. Manjóna
Pressure-induced order-disorder transitions in β-In2S3: an experimental and theoretical study of structural and vibrational properties
Physical Chemistry Chemical Physics 23, 23625 (2021).

999. D. Singh and R.Ahuja
Polypeptoid material as an anchoring material for Li-S batteries
ACS Applied Energy Materials **4,** 13070 (2021).

1000. D.Singh and R.Ahuja,
A Theoretical Prediction of Bi-doped β-Antimonene Monolayer as a Highly Efficient Photocatalysts for Oxygen Reduction and Overall Water Splitting
ACS Applied Materials & Interfaces 13, 56254 (2021).

1001. P. Sharma, Pratigya; M. Sundaram, T. Watcharatharapong, S. Jungthawan and R. Ahuja, Tuning the nanoparticle interfacial properties and stability of core-shell structure in Zn Doped NiMoO4@AWO4
ACS Applied Materials & Interfaces 13, 56116 (2021).

1002. H. Li, T. Duan, O. Sher, Y. Han, R. Papadakis, A. Grigoriev, R. Ahuja and K. Leifer, Fabrication of BP2T functionalized graphene via non-covalent π-π stacking interactions for enhanced ammonia detection
RSC Advances 11, 35982 (2021).

1003. D. Kumar, J. Kaur, P.P. Mohanty, R. Ahuja and S. Chakraborty,
Recent Advancements in Non-toxic Halide Perovskites: Beyond Divalent Composition Space
ACS Omega 6, 33240 (2021).

1004. N. Vats, D. S Negi, D. Singh, W. Sigle, S. Abb, S. Sen, S. Szilagyi, H. Ochner, R. Ahuja, K. Kern, S. Rauschenbach, P. A van Aken
Catalyzing Bond-Dissociation in Graphene via Alkali-Iodide Molecules
Small 17, 2102037(2021).

1005. M. Rkhis, S. Laasri, S. Touhtouh, E-K. Hlil, M. Bououdina, R. Ahuja and A. Hajjaji, Engineering the hydrogen storage properties of the Perovskite hydride ZrNiH3 by uniaxial/biaxial strain
International Journal of Hydrogen Energy 47, 3022(2022).

1006. S. Mishra, E. Jeanneau, L. Tian, I. Nuta, E. Blanquet, D. Singh, R. Ahuja, C. Marichy and S. Daniele,
Asymmetry-Induced Redistribution in Sn(IV)-Ti(IV) Heterobimetallic Alkoxide Precursors and its Impact on Thin Films Deposition by MOCVD
Crystal Growth & Design 22, 54 (2022).

1007. M Ye, Y Teng, X Zhao, S Wang, J Tang, R Ahuja
Preparation and characterization of SiC-ZAC composite material for immobilizing the simulated radioactive graphite
Progress in Nuclear Energy 143, 104029 (2022).

1008. M. Zidane, E. Salmani, A. Majumdar, M. Elmoulat, M. Bghour, A. Labrag, H. Ez-Zahraou, A. Benyoussef and R. Ahuja
Thermophysical properties of Helium and Hydrogen mixtures under high pressure predicted by ab-initio calculations: implications for Saturn and Jupiter planets
Chemical Physics 555, 111430 (2022).

1009. P. Panigrahi, M. Sajjad, D. Singh, T. Hussain, J. A. Larsson, R. Ahuja & N. Singh
Two-Dimensional Nitrogenated Holey Graphene (C2N) Monolayer Based Glucose Sensor for Diabetes Mellitus
***Applied Surface Science* 573,** 151579 (2022).

1010. M. Ye, Y. Teng, X. Zhao, S. Wang, J. Tang, H. Liu, X. Zheng, A. T. Rasulovich & R. Ahuja
Preparation and Properties of Situ-sintered SiC Ceramics aided by ZnO-Al2O3-CaO
Journal of Alloys and Compounds 890, 161854 (2022).

1011. X. Zhao, Y. Li, Y. Teng, H. Liu, X. Zheng, H. He, S. Wang and R. Ahuja,
Exploring the relationship between Ln leaching and Ln-O binding energy in monazite (Nd, Sm, Eu)
***Journal of the American Ceramic Society* 105,** 553 (2022).

1012. H.R. Mahida, A. Patel, D. Singh, Y. Sonvane, P.B. Thakor and R.Ahuja
First-principles calculations to investigate electronic structure and optical properties of 2D MgCl2 monolayer
Superlattices and Microstructures 162, 107132(2022).

1013. W. Sukmas, P. Tsuppayakorn-aek, U. Pinsook, R. Ahuja and T. Bovornratanaraks
Roles of Optical Phonons and Logarithmic Profile of Electron-Phonon Coupling Integration in Superconducting Sc0.5Y0.5H6 Superhydride Under Pressures
Journal of Alloys and Compounds 901, 163524 (2022).

1014. D. Singh and R.Ahuja,
Dimensionality effects in high-performance thermoelectric materials: computational and experimental progress in energy harvesting applications
***WIREs Computational Molecular Science* 12,** e1547 (2022).

1015. A. Majumdar & R.Ahuja
Pressure Induced Structural Phase Transition and Piezochromism in Photovoltaic Sillen Compounds PbBiO2X (X = Cl, Br & I)
***Applied Materials Today* 26,** 101372 (2022).

1016. H. Gou, S. Zhao, S. Xu, J. Yao, N. Chen, Y. Gong, X. Zhang, X. Hao, L. Zhang, C. Pei, R. Tian, L. Wu, B. Wan, W. Peng, B. Gao, Y. Qi, F. Gao, R. Ahuja and Y. Yao

Elucidating the Reaction Pathway of Crystalline Multi-metal Borides for Highly Efficient Oxygen-Evolving Electrocatalysts
Journal of Materials Chemistry A 10, 1569 (2022).

1017. S. Deshpande, M. Deshpande, T. Hussain and R. Ahuja,
Binding and Optical Characteristics of Polycyclic Aromatic Hydrocarbons and their Nitroderivatives adsorbed C3N Monolayer
***New Journal of Chemistry* 46,** 2245 (2022).

1018. P. K. Panda, D. Singh, M. H. Köhler, D. D. de Vargas, Z. L. Wang and R. Ahuja
Contact Electrification through Interfacial Charge Transfer: A Mechanistic Viewpoint on Solid-liquid interface
***Nanoscale Advances* 4,** 884 (2022).

1019. A. N. Rao, N. P. M. J. Raj, G. Khandelwal, P. K. Panda, A. Banerjee, Y. K. Mishra, R. Ahuja and S. J. Kim
Crystallinity modulation originates ferroelectricity like nature in piezoelectric selenium
***Nano Energy* 95,** 107008 (2022).

1020. P. K. Panda, P. Kumari, P. Patel, S. K. Samal, S. Mishra, M. M. Tambuwala, A. Dutt, K. Hilscherova, Y. K. Mishra, R. S. Varma, M. Suar, R. Ahuja and S. K. Verma
Molecular nanoinformatics approach assessing the biocompatibility of biogenic silver nanoparticles with channelized intrinsic steatosis and apoptosis
Green Chemistry 24, 1190 (2022).

1021. E. Anikina, S. R. Naqvi, H. Bae, H. Lee, W. Luo, R. Ahuja and T. Hussain
High-Capacity Reversible Hydrogen Storage Properties of Metal-Decorated Nitrogenated Holey Graphenes
International Journal of Hydrogen Energy 47, 10654 (2022).

1022. D.Raval, S.K. Gupta, P.N.Gajjar and R.Ahuja
Strain Modulating Electronic Band Gaps and SQ Efficiencies of Semiconductor 2D PdQ2 (Q= S, Se) monolayer
Scientific Reports 12, 2964 (2022).

1023. M. Behloul, Y. Benhouria, H. Ez-Zahraouy, I. Essaoudi, A. Ainane and R. Ahuja
Electronic and magnetic behaviors of (V, Mn), (V, Fe) and (V, Cu) codoped tin carbide: Ab initio and Monte Carlo calculations
Materials Today : Proceedings 53, 448 (2022).

1024. I. Hussain, T. Hussain, M. Ahmad, X. Ma, M.S. Javed, C. Lamiel, R. Ahuja, Y.Chen and K. Zhang,
Modified KBBF-like Material for Energy Storage Applications: $ZnNiBO_3(OH)$ with Enhanced Cycle Life
ACS Applied Materials & Interfaces 14, 8025 (2022).

1025. D.Singh and R.Ahuja
Two-dimensional perovskite/HfS_2 vdW heterostructure as an absorber material for photovoltaic applications
ACS Applied Energy Materials 5, 2300 (2022).

1026. A.K. Jena, S.K. Mallik, M.C. Sahu, S. Sahoo, A. Sahoo, J.R. Mohanty, S. Gupta, R. Ahuja and S. Sahoo,
Strain-mediated Ferromagnetism and Low-field Magnetic Reversal in Co Doped Monolayer WS_2
Scientific Reports volume 12, 2593 (2022).

1027. A. Ghosh, D. Singh, Q. Mu, Y. Kvashnin, G. Haider, M. Jonak, D. Chareev, T. Aramaki, S. A. Medvedev, R. Klingeler, M. Mito, E. H. Abdul-Hafidh, J. Vejpravova, M. Kalbac, R. Ahuja, O. Eriksson and M. Abdel-Hafiez
Exotic magnetic and electronic properties of layered CrI 3 single crystals under high pressure
Physical Review B (Letter) 105, L081104 (2022).

1028. P. Panigrahi, P.K. Panda, Y.Pal, H. Bae, H. Lee, R. Ahuja and T. Hussain
Two-Dimensional Bismuthene Nanosheets for Selective Detection of Toxic Gases
ACS Applied Nano Materials 5, 2984 (2022).

1029. A. Nair, A. Anoop, R. Ahuja and B. Pathak,
Relativistic Effects in Platinum Nanocluster Catalysis: A Statistical Ensemble Based Analysis
The Journal of Physical Chemistry A 126, 1345(2022).

1030. N. Khossossi, W. Luo, Z. Haman, D. Singh, I. Essaoudi, A. Ainane and R. Ahuja
Revealing the superlative electrochemical properties of o-B2N2 monolayer in Lithium/Sodium-ion batteries
Nano Energy 96, 107066 (2022).

1031. D. Singh, . N. Khossossi, W. Luo, A. Ainane and R. Ahuja
2D Janus and non-Janus diamanes with an in-plane negative Poisson's ratio for energy applications
Materials Today Advances 14, 100225 (2022).

1032. N. K. Sharma, S. Sahoo, M. C. Sahu, S. K. Mallik, A. K. Jena, H. Sharma, S. Gupta, R. Ahuja and S. Sahoo
Electronic Bandstructure Modulation of MoX2/ZnO(X:S,Se) Heterostructure by Applying External Electric Field
Surfaces and Interfaces 29, 101817 (2022).

1033. Z. Haman, N. Khossossi, M. Kibbou, I. Bouziani, D. Singh, I. Essaoudi, A. Ainane and R. Ahuja
Janus Aluminum Oxysulfide Al2OS: A promising 2D direct semiconductor photocatalyst with strong visible light harvesting
Applied Surface Science 589, 152997 (2022).

1034. S. Gupta, P. K. Panda, R. Hashimoto, S. Samal, S. Mishra, S. K. Verma, Y. Mishra and R. Ahuja
Dynamical modeling of miR-34a, miR-449a, and miR-16 reveals numerous DDR signaling pathways regulating senescence, autophagy, and apoptosis in HeLa cells
Scientific Reports 12, 4911 (2022).

1035. Q Hu, J Tang, Y Teng, X Zhao, T Arslanov and R Ahuja
Preparation and dielectric properties of La doped NBCCTO ceramics
***Journal of Electroceramics* 48,** 117 (2022).

1036. S. Bahtia, M. Kibbou, N. Khossossi, I. Essaoudi, A. Ainane and R. Ahuja,
Structures, Stabilities, Optoelectronic and Photocatalytic properties of Janus Aluminium mono-chalcogenides Al(Ga, In)STe monolayers
Physica E 142, 115229 (2022).

1037. H. Liu, X. Zhao, Y. Teng, Y. Li, X. Zheng, S. Wang, L. Wu, P. K. Panda and R. Ahuja
Investigation of Nd3+ incorporation in Ce-Rhabdophane: Insight from structural properties and occupation mechanism
Journal of the American Ceramic Society 105, 4974 (2022).

1038. S. Samal, P. K. Panda, M. Vikström, K. Leander, U. de Faire, R. Ahuja and J. Frostegard
Antibodies against Phosphorylcholine Among 60-Year-Olds: clinical role and simulated interactions
Frontiers in Cardiovascular Medicine 9, 809007 (2022).

1039. P. Tsuppayakorn-aek, N. Phaisangittisakul, R. Ahuja and T. Bovornratanaraks
Stabilizing superconductivity of ternary metal pentahydride $CaCH_5$ via electronic topological transitions under high pressure from first principles evolutionary algorithm
Scientific Reports 12, 6700 (2022).

1040. P. Mishra, D. Singh, Y. Sonvane and R. Ahuja
Bifunctional Catalytic Activity of 2D Boron Monochalcogenides BX (X = S, Se, Te)
Materials Today Energy 27, 101026 (2022).

1041. P. P. Mohanty, R. Ahuja and S. Chakraborty
Progress and Challenges in Layered Two-dimensional Hybrid Perovskites
Nanotechnology 33, 292501 (2022).

1042. P. Pluengphon, P. Tsuppayakorn-aek, R. Ahuja and T. Bovornratanaraks
TM dopant-induced H-vacancy diffusion kinetics of sodium-lithium alanates: Ab initio study for hydrogen storage improvement
International Journal of Hydrogen Energy 47, 18763 (2022).

1043. K. Gaurav, B. SanthiBhushan, G. Gutierrez, Rajeev Ahuja and A. Srivastava
Trans-polyacetylene Based Organic Spin Valve for a Multifunctional Spin-Based Device: A First Principle Analysis

Journal of Science: Advanced Materials and Devices 7, 100459 (2022).

1044. N. Khossossi, D. Singh, W. Luo and R. Ahuja
Flexible 3D porous boron nitride interconnected network as a high-performance Li-and Na-ion battery electrodes
Electrochimica Acta 421, 140491 (2022).

1045. M.Kibbou, Z. Haman, N. Khossossi, D. Singh, I. Essaoudi, A. Ainane and R.Ahuja
Probing the electronic, optical and transport properties of halide double perovskites Rb2InSb(Cl,Br)6 for solar cells and thermoelectric applications
Journal of Solid State Chemistry 312, 123262 (2022).

1046. A**.** Nath, R. Bhattacharjee, A. Nandi, A. Sinha, S. Kar, N. Manoharan, S. Mitra, A. Mojumdar, P. K. Panda, S. Patro, A. Dutt, R. Ahuja, S. K. Verma and M. Suar
Phage delivered CRISPR-Cas system to combat multidrug-resistant pathogens in gut microbiome
Biomedicine & Pharmacotherapy 151, 113122 (2022).

1047. V.T. Phuc, P.T.B. Thao, R. Ahuja and N.T. Tien
Effect of phosphorus doping positions on electronic transport properties in the sawtooth penta-graphene nanoribbon: First-principles insights
Solid State Communications 353, 114859 (2022).

1048. P. Panigrahi, Y. Pal, D. Raval, S. K. Gupta, P. N. Gajjar, H. Bae, H. Lee, S. Mark, R. Ahuja, R. Pandey and T.Hussain
Tuning the Selective Sensing Properties of Transition Metal Dichalcogenides (MoX2: X= Se, Te) Towards Sulfur Rich Gases
***Materials Today Chemistry* 26,** 101069 (2022).

1049. G.A. Shaikh, D. Cornil, S.K. Gupta, R. Ahuja and P.N. Gajjar
Prominent Electrode Material for Na-, K-, and Mg-ion Batteries: 2D β-Sb Monolayer
Energy & Fuels 36, 7087(2022).

1050. A. Allal, M. Halit, S. Saib, W. Luo and R. Ahuja
Phase stability, phonon, electronic, and optical properties of not-yet-synthesized CsScS2, CsYS2, and APmS2 (A= Li, Na, K, Rb, Cs) materials: insights from first-principles calculations
Materials Science in Semiconductor Processing 150, 106936 (2022).

1051. S. K. Mallik, S. Sahoo, M. C. Sahu, N. K. Sharma, A. K. Jena, S. K. Gupta, R. Ahuja and S. Sahoo
Transition Metal Substituted MoS2/WS2 van der Waals Heterostructure for Realization of Dilute Magnetic Semiconductors
Journal of Magnetism and Magnetic Materials 560, 169567 (2022).

1052. A.Benerjee, N. Khossossi, W.Luo and R.Ahuja
Promise and reality of organic electrodes from materials design and charge storage perspective
Journal of Materials Chemistry A 10, 15215 (2022).

1053. P. Tsuppayakorn-aek, R. Ahuja, T. Bovornratanaraks and W. Luo
Superconducting Gap of Pressure Stabilized $(Al_{0.5}Zr_{0.5})H_3$ from ab initio Anisotropic Migdal-Eliashberg Theory
ACS Omega 7, 28190 (2022).

1054. S. Deshpande, M. Deshpande, R. Ahuja and T. Hussain,
Tuning the Electronic, Magnetic, and Sensing Properties of Single Atom Embedded Microporous C_3N_6 Monolayer Towards XO_2 (X=C,N,S) Gases
New Journal of Chemistry 46, 13752(2022).

1055. A. Patel, D. Singh, Y. Sonvane, P.B. Thakor and R. Ahuja
Optoelectronic properties of 2D van der Waals heterostructure As/PtS2 by first-principles calculations
Accepted for publication in ***Materials Today Proceedings.***

1056. K. Kotmool, T. Kaewmaraya, T. Hussain, R. Ahuja, W. Luo and T. Bovornratanaraks,
Biaxial stress and functional groups (T = O, F, and Cl) tuning structural, mechanical, and electronic properties of monolayer molybdenum carbide
Physical Chemistry Chemical Physics 24, 17862 (2022).

1057. P. Sharma, D. Singh, M. Minakshi, S. Quadsia and R. Ahuja
Activation-Induced Surface Modulation of Biowaste-Derived Hierarchical Porous Carbon for Supercapacitors
Accepted for publication in ***ChemPlusChem.***

1058. J. Deb, R. Ahuja and U. Sarkar
Two-Dimensional Pentagraphyne as a High-Performance Anode Material for Li/Na-Ion Rechargeable Batteries
Accepted for publication in ***ACS Appl. Nano Mater.***

1059. P. Tsuppayakorn-aek, T. Bovornratanaraks , R. Ahuja, T. Bovornratanaraks & W. Luo,
Existence of yttrium allotrope with incommensurate host–guest structure at moderate pressure: First evidence from computational approach, ***Computational Materials Science 213,*** 111652 (2022).

1060. X. Zhao, Y. Tenga, Y. Li, X. Zheng, Q. Zheng, R. Ma, G. Liu, Y. Liu, R. Ahuja and Wei Luo,
Response of Nd3+ and Sm3+ Precipitating into Rhabdophane and the Leaching Mechanism of Associated Monazite Ceramics,
Accepted for publication in ***Journal of the American Ceramic Society.***

1061. S. Gupta, P. Panda, R. Hashimoto, W.Luo and R. Ahuja.
Network Analysis Reveals that the Tumor Suppressor lncRNA GAS5 Acts as a Double-edged Sword in response to DNA damage in Gastric Cancer
Accepted for publication in ***Scientific Reports.***

1062. A. K. Bhojani, H. L Kagdada, R. Ahuja and D. K. Singh
Carbon-based Monochalcogenides for Efficient Solar and Heat Energy Harvesting
Accepted for publication in ***Applied Surface Science.***

1063. S. Singh, D. Singh, R. Ahuja, M. Fichtner and P. Barpanda,
Eldfellite NaV(SO4)2 as a versatile cathode insertion host for Li-ion and Na-ion batteries
Accepted for publication in ***Journal of Materials Chemistry A.***

1064. R. Gond, S. Singh, X. Zhao, D. Singh, R. Ahuja, M. Fichtner and P. Barpanda,
Pyrophosphate Na2CoP2O7 Polymorphs as Efficient Bifunctional Oxygen Electrocatalysts for Zinc-Air Batteries
Accepted for publication in ***ACS Applied Materials & Interfaces.***

1065. D. Gupta, A. Kafle, S. Kaur, P. P. Mohanty, T. Das, S. Chakraborty, R. Ahuja and T. Nagaiah,
High yield selective electrochemical conversion of N2 to NH3 via morphology controlled silver phosphate under ambient conditions
Accepted for publication in ***Journal of Materials Chemistry A.***

1066. Q. Hu, Y. Teng, X. Zhao, T. Arslanov, Q. Zheng, T. Luo, R. Ahuja and W. Luo
Temperature stable dielectric properties of Mg2TiO4-MgTiO3-CaTiO3 Ceramics Over a Wide Temperature range
Accepted for publication in ***Ceramics International.***

1067. D. de Vargas, G. L. Cardoso, P. Piquini, R. Ahuja and R. Baierle
2D Dumbbell Silicene as High Storage Capacity and Fast Ion Diffusion Anodes for Li-Ion Batteries
Accepted for publication in ***ACS Applied Materials & Interfaces.***

1068. I. Jason, Y. Pal, P. Anees, H. Bae, H. Lee, R. Ahuja, T. Hussain and P. Panigrahi
Superalkali Functionalized Two-Dimensional Haeckelite Monolayers: A Novel Hydrogen Storage Architecture
Accepted for publication in ***International Journal of Hydrogen Energy.***

1069. P. Panigrahi, Y. Pal, A. Panigrahi, H. Bae, H. Lee, R. Ahuja and T. Hussain
Efficient Sensing of Selected Amino Acids as Biomarker by Green Phosphorene Monolayers: Smart Diagnosis of Viruses
Accepted for publication in ***Advanced Theory and Simulations.***

1070. D. Singh, V. Shukla, N. Khossossi, P.Hyldgaard and R.Ahuja
Stability of and conduction in single-walled Si 2BN nanotubes
Accepted for publication in ***Physical Review Materials.***