Dr. Vivekanand Shukla

Résumé

Contact Information

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Personal Data

Date of Birth: July 05^{th}, 1988 Marital status: Married

Work Experience

06/2023-present **Indian Institute of Technology Ropar**, Department of Physics, India
Assistant Professor
Principle Investigator: Computational Materials Physics Laboratory

08/2022-05/2023 **Technical University Dresden**, Chair of Theoretical Chemistry, Germany
10 months Postdoctoral Fellow with Prof. Thomas Heine

Current research focuses on the nature of the heterostructures (HSs) formed from novel magnetic 2D materials and the new physical phenomena they offer, bearing the potential of a transformative impact. The plan is to investigate HSs of 2D antiferromagnetic (AFM) semiconductors with valley-polarized transition metal dichalcogenides or/and 2D superconductors. We aim to control the HS properties by tuning the strength and nature of interlayer interactions due to rotational alignment, interlayer charge transfer, and electronic characteristics of the layers. Ultimately, with our experimental collaborators, the accumulated knowledge on 2D HSs will be harnessed toward demonstrating a working paradigm of novel quantum optoelectronic devices.

05/2021-06/2022 **Chalmers University of Technology**, EMS Laboratory, Microtechnology & Nanosciences, Gothenburg, Sweden, 1 year 2 months
Researcher with Prof. Per Hyldgaard

05/2019-04/2021 **Chalmers University of Technology**, EMS Laboratory, Microtechnology & Nanosciences, Gothenburg, Sweden, 2 years
Postdoctoral Fellow with Prof. Per Hyldgaard

My research was focused on resolving important remaining challenges for the organics-interface problem and for asserting the vdW-DF method's potential for a truly parameter-free exploration of biochemistry problems. The project included implementation work and facilitation of first-principles DFT studies of organic systems. In addition, I also worked on building trust in the method by defining and launching new experiment-based benchmarking suits that are relevant for future biochemistry and organic metal interfaces. This work involves analysis and method development and code implementation for nonlocal DFT, as well as work to define and launch new benchmarking.

Education

09/2014-02/2019 **Doctor of Philosophy** in Physics, Uppsala University, Department of Physics & Astronomy, Uppsala, Sweden.
Doctoral Thesis: "Computational Studies of 2D Materials: Application to Energy Storage and Electron Transport in Nanoscale Devices" [link].
Adviser: Prof. Rajeev Ahuja

07/2012-06/2014 **Master of Technology** in Material Science, Indian Institute of Technology Kanpur, Samtel Centre for display technologies, India

	Thesis: "Graphitic Carbon Nitride (g-C_3N_4): Synthesis and characterization of bulk and thin films for device applications" [link]. Adviser: Prof. Y. N. MOHAPATRA
08/2009-07/2011	**Master of Science** in PHYSICS, Major: Electronics, Deen Dayal Upadhyaya Gorakhpur University, Gorakhpur, INDIA
07/2006-06/2009	**Bachelor of Science** (MATH, PHYSICS & CHEMISTRY), Deen Dayal Upadhyaya Gorakhpur University, Gorakhpur, INDIA

SCHOLASTIC ACHIEVEMENTS

06/2019	Best poster prize (EMMC-eSSENCE meeting with the sub-theme of physics based data-driven modelling) eSSENCE Multiscale Modelling Meeting, Uppsala, Sweden
09/2017	Anna Maria Lundin's Travel Grant (To attend the MRS 2017 Fall meeting in Boston USA)
06/2014	Erasmus Mundus (NAMASTE Consortium Grant). (European Union scholarship for Doctoral study in Uppsala University Sweden)
07/2012	Junior Research Fellowship (JRF) (University Grant Commission, Govt. of India)
03/2012	Graduate Aptitude test Engineering **(GATE)**, All India Rank **216** (Ministry of Human Resource and Development,Govt. of India)
08/2012	National Eligibility Test, All India Rank **192** (Council of Scientific and Industrial Research, Govt. of India)
07/2009	Masters in Science Admission test (Conducted by St. Andrews College Gorakhpur, Gorakhpur, India)

SCIENTIFIC RESEARCH INTERESTS

Broad

- Extensive academic research experience in the field of Theoretical and Computational Material Science involving diverse class of materials using state of the art density functional theory, quantum mechanical, multi-scale materials modelling and method development.

Specific

- Development and bench-marking of non-local density functional vdW-DF.
- Study of surface adsorption, interface and edge effects.
- Gas sensing activities, edge effects, functionalization of 2D materials.
- Electronic, magnetic and transport properties of 2D materials and heterostructures.
- Materials modeling for energy applications.
- Electronic and structural properties of materials at extreme conditions.
- Optoelectronic and Thermoelectric properties of materials.

COMPUTATIONAL SKILLS

SOFTWARE

- Experience working with Quantum ESPRESSO, VASP, SIESTA, TranSIESTA, WIEN2k, GPAW, INELASTICA. LOBSTER, ENVIRON, ASE, ACONVASP
- Intermediate skills in Gaussian, Phonopy
- Expert in code optimization, and benchmarking on high performance computing infrastructure.

Method development

- Implementation and benchmarking the range separated hybrid functionals vdW-DF-ahcx and vdW-DF2-ahbr [link], [link]
  Available in open access code Quantum Espresso 7.0
- PPACF library: Helped in testing and maintenance of the PPACF code library
  Available in Quantum Espresso for post processing [link]

Programing Languages

- Proficient in using Python, Shell Scripts, Matlab, LaTeX.
- Familiarity with Fortran

Participation in organizations & other professional activities

Teaching

- Department of Physics, IIT Ropar, India
  Semicondcutor Physics (Spring 2023-2024)
- Department of Physics, IIT Ropar, India
  Incharge and Set up a laboratory for Engineering Physics undergraduate course (Fall 2023-2024)
- Department of Physics and Astronomy, Uppsala University, Sweden
  Quantum Physics Laboratory for undergraduate students
  (Fall 2016-17, Spring 2017)
- Materials Science Program, IIT Kanpur, India (Fall 2013)
  Characterization of Materials Laboratory, M.Tech 1^{st} year students.
- Sardar Patel Institute of Science and Technology Gorakhpur, India
  Quantum Mechanics for undergraduate students
  (Visiting lecturer 2011-12)

Supervision

- Masters Thesis supervision **Ashutosh Kinikar**, 2020
  Chalmers University of Technology, Gothenburg, Sweden
  Thesis title: *A vdW density functional study of a DNA base-pair duplex*
- PhD Thesis supervision **Carl Mikael Frostenson**, **Ongoing**,
  Chalmers University of Technology, Gothenburg, Sweden

Conferences and Workshops

Contributed talks

- Invited talk, Technical University Dresden, Dresden, Germany, June 2022
- Invited talk, Institute of Nano Science and Technology, Mohali, India, April 2022
- APS March Meeting, Chicago, March 14–18, 2022
- Invited talk, Indian Institute of Technology Ropar, India, Feb 2022
- Webinar series on recent development in materials science, St. Andrews College Gorakhpur, 2020
- Invited talk, Chalmers University of Technology, Sweden 2019
- Area of Advance symposium, Chalmers University of Technology, Sweden 2019
- Uppsala (VR-Sweden)-Dalian (NSFC-China) symposium on Materials for Energy Applications, Uppsala, Sweden 2019
- Materials Research Society, Fall Meeting, Boston, USA 2017

Poster presentations

- MOLECULAR FOUNDRY USER MEETING; A nanoscience conference at Lawrence Berkeley National Laboratory, 08/2020
- EMMC-eSSENCE meeting with the sub-theme of physics based & data-driven modelling,
  eSSENCE Multiscale Modelling Meeting, Sweden, 06/21
- EI Nano and graphene center conference Community Building,
  EI Nano Community Building, Sweden, 08/19

- Best Poster Prize: EMMC-eSSENCE meeting with the sub-theme of physics based & data-driven modelling,
  eSSENCE Multiscale Modelling Meeting, Sweden, 06/19
- Yambo workshop at CECAM-HQ-EPFL, Lausanne, Switzerland, 2015
- Multi-electrode nanoscale transport with non-equilibrium Green's Functions: From tight-binding to DFT **DTU**, Denmark, 10/17
- **ASE** workshop in Chalmers University of Technology, Sweden, 11/19

Synergistic Activities

2015 – 2017 Information Officer – TNDR Board (The PhD student's council of the faculty of science and technology, Uppsala University)

2010 – 2011 Served as President of Physics Association at St. Andrews College Gorakhpur

Publications & Preprints

Summary

- **25 published papers 12 as a first author**
- Including: Physical review X = 1 (1^{st} author), Nano energy = 2 (1^{st} author), ACS-AMI = 2 (one as a 1^{st} author), PCCP = 2 (1^{st} author), JPC-C= 1 (1^{st} author), Phys Rev B = 1, Physical Review Materials = 1 (Joint 1^{st} author), Inorganic Chemistry = 1, PNAS = 1, Applied Surface Science = 1, Nanoscale = 1, Nanoscale Advances = 1 (1^{st} author), New Journal of Chemistry = 1, Applied Materials Today = 1, Materials Today Bio = 1, Advanced Theory & Simulations = 1, ACS Applied Energy Materials = 1, JCPM = 1 (1^{st} author), ACS Applied Electronic Materials = 1 (1^{st} author), Electronic Structure = 1; 2 Review articles: JPCM =1, JP: energy (Joint 1^{st} author), 2 manuscript submitted and 3 manuscripts under preparation
  No. of citations = **950+**(Google Scholar), h-index = **16**, i10-index = **21**

Peer Reviewed Articles

25. Physical Review X, **12**, 041003, (2022) [link]
    V Shukla, Y jiao, J-H Lee, E Schroder, J B Neaton, P Hyldgaard, *Accurate nonempirical range-separated hybrid van der Waals density functional for complex molecular problems, solids, and surfaces*

24. Physical Review Materials, **6**, 116001, (2022)[link]
    D Singh*, **V Shukla***, N Khosossi, P Hyldgaard, R Ahuja, *Stability of and conduction in single-walled Si_2BN nanotubes* (Joint first and main corresponding author)

23. Electronic Structure, **4**, 014001, (2022) [link]
    C M Frostenson, E J Granhed, **V Shukla**, Pär AT Olsson, E Schroder, P Hyldgaard, *Hard and soft materials: Putting consistent van der Waals density functionals to work*

22. Journal of Physics: Condensed Matter **34**, 025902 (2021) [link]
    V shukla, Y jiao, C frostenson, P Hyldgaard, *vdW-DF-ahcx: a range-separated van der Waals density functional hybrid*

21. ACS Applied Electronic Materials 2021 **3**, 733-742 (2021) [link]
    V Shukla, R L Kumawat, N K Jena, B Pathak, R Ahuja, *Electronic and Transport Properties of Bilayer Phosphorene Nanojunction: Effect of Paired Substitution Doping*

20. Journal of Physics: Energy (Topical Review), **3**, 012005 (2020) [link]
    D Singh*, **V Shukla***, N Khosossi*, A Ainane, R Ahuja, *Harnessing the unique properties of MXenes for advanced rechargeable batteries* (Joint first author)

19. Physical Review B **102**, 075444 (2020) [link]
D Singh, **V Shukla**, R Ahuja, *Optical excitations and thermoelectric properties of two-dimensional holey graphene*

18. Advanced Theory and Simulations **3**, 2000023 (2020) [link]
N Khossossi, **V Shukla**, Y Benhouria, I Essaoudi, A Ainane, & R Ahuja , *Exploring the Possibility of β-Phase Arsenic-Phosphorus Polymorph Monolayer as Anode Materials for Sodium-Ion Batteries*

17. ACS Applied Energy Materials **3**, 7306 (2020) [link]
N Khossossi, P Panda, D Singh, **V Shukla**, Y Mishra, I Essaoudi, A Ainane & R Ahuja *Rational Design of 2D h-BAs Monolayer as Advanced Sulfur hosts for High Energy Density Li-S Batteries*

16. Journal of Physics: Condensed Matter (Topical Review) **32**, 393001 (2020) [link]
P Hyldgaard, Y Jiao, **V Shukla**, *Screening nature of the van der Waals density functional method: a review and analysis of the many-body physics foundation*

15. Nanoscale Advances **2**, 1493 (2020) [link]
V Shukla, A Grigoriev, R Ahuja, *Rectifying behavior in twisted bilayer black phosphorus nanojunctions mediated through intrinsic anisotropy*

14. Applied Materials Today **19**, 100574 (2020) [link]
S R Naqvi, **V Shukla**, N K Jena, W Luo, R Ahuja, *Exploring two-dimensional M_2NS_2 (M= Ti, V) MXenes based gas sensors for air pollutants*

13. New Journal of Chemistry **44**, 3777 (2020) [link]
D Singh, **V Shukla**, P K Panda, Y K Mishra, H Rubahn, R Ahuja, *Carbon-Phosphide Monolayer with High Carrier Mobility and Perceptible I-V Response for Superior Gas Sensing*

12. Applied Surface Science **497**, 143660 (2019) [link]
J Prasongkit, **V Shukla**, A Grigoriev, R Ahuja, V Amornkitbamrung, *Ultrahigh-sensitive gas sensors based on doped phosphorene: A First-principles investigation*

11. Nano Energy **58**, 877 (2019) [link]
V Shukla, N K Jena, S R Naqvi, W lou, R Ahuja, *Modeling High-performing Batteries with MXenes: The case of S-functionalized two-dimensional Nitride MXene Electrode*

10. Materials Today Bio **1**, 100001 (2019) [link]
S Umrao, A K Maurya, **V Shukla**, A Grigoriev, R Ahuja, M Vinayak, R R Srivastava, P S Saxena, I Oh, A Srivastava, *Anticarcinogenic activity of blue fluorescent hexagonal boron nitride quantum dots: as an effective enhancer for DNA cleavage activity of anticancer drug doxorubicin*
(First author from the theory side)

9. Nanoscale **11**, 6571 (2019) [link]
I H Wani, SHM Jafri, J Wärnå, A Hayat, H Li, **V Shukla**, A Orthaber, A Grigoriev, R Ahuja, K Leifer, *A sub 20 nm metal-conjugated molecule junction acting as a nitrogen dioxide sensor*

8. Physical Chemistry Chemical Physics **20**, 22008 (2018) [link]
V Shukla, R B Araujo, N K Jena, R Ahuja, *Borophene's Tryst with Stability: Exploring 2D Hydrogen Boride as Electrode for Rechargeable Batteries*

7. Physical Chemistry Chemical Physics **20**, 22952 (2018) [link]
V Shukla, A Grigoriev, N K Jena, R Ahuja, *Strain controlled electronic and transport anisotropies in two-dimensional borophene sheets*

6. The Journal of Physical Chemistry C **121** 26869 (2017) [link]
V Shukla, J Warna, N K Jena, A Grigoriev, R Ahuja, *Toward the realization of 2D borophene*

based gas sensor

5. ACS applied materials & interfaces **9**, 39945 (2017) [link]
   V Shukla, N K Jena, A Grigoriev, R Ahuja, *Prospects of Graphene–hBN Heterostructure Nanogap for DNA Sequencing*

4. Nano Energy **41**, 251 (2017) [link]
   V Shukla, R B Araujo, N K Jena, R Ahuja, *The curious case of two dimensional Si_2BN: A high-capacity battery anode material*

3. ACS applied materials & interfaces **9**, 16148 (2017) [link]
   N K Jena, R B Araujo, **V Shukla**, R Ahuja, *Borophane as a benchmate of graphene: a potential 2D material for anode of Li and Na-ion batteries*

2. Inorganic chemistry **56**, 5918 (2017) [link]
   R Gond, S S Meena, S M Yusuf, **V Shukla**, N K Jena, R Ahuja, S Okada, P Barpanda, *Enabling the Electrochemical Activity in Sodium Iron Metaphosphate $[NaFe(PO_3)_3]$ Sodium Battery Insertion Material: Structural and Electrochemical Insights*
   (First author from the theory side)

1. Proceedings of the National Academy of Sciences **114**, 3596 (2017) [link]
   C Ji, A F Goncharov, **V Shukla**, N K Jena, *et al.*, *Stability of $Ar(H_2)_2$ to 358 GPa*
   (First author from the theory side)

Manuscript submitted to journal

1. Under Review in Physical Review Materials
   R. Hissariya, **V Shukla**, N. Tripathi, T. Brumme, & S. K. Mishra, *Antisite disorder induced exchange bias and spin-glass state in $La_{1.5}Sm_{0.5}NiMnO_6$* (First author from the theory side)

2. Under Review in ACS Applied Nano Materials
   R L Kumawat*, **V Shukla***, N K Jena, R Ahuja, and B Pathak *The Merits of Folded Graphene Nanogap for Reliable DNA Sequencing* (Joint first and corresponding author)

Manuscript under preparation

1. **V Shukla**, Per Hyldgaard
   Revisiting CO adsorption puzzle: Role of accurate density and nonlocal correlation

2. **V Shukla**, P Hyldgaard
   Assessment of hybrid van der Waals (vdW-DFs) functionals: bandgap of solids

3. **V Shukla***, R L Kumawat*, R Ahuja, B Pathak
   Effect of Stacking Twisting Electric field and Mechanical Strain on Black Arsenene

Review activities

Reviewing for
- Nature Electronic (Nature group), JPCM & Nanotechnology (IOPscience), PCCP & Nanoscale (RSC), Applied Surface Science & Computation Materials Science, (Elsevier), etc.

Associate editor
- Frontiers in Energy Research a MDPI Journal

Punjab, India, May, 2024 — Vivekanand Shukla