

CONTACT INFORMATION

Institute of Theoretical Physics and Astrophysics
University of Kiel
Leibnizstraße 15
D-24098 Kiel
Germany

MOBILE: +49 171 5604142
EMAIL: haldar@physik.uni-kiel.de
haldar.physics@gmail.com
PUBLICATION: [Google Scholar](#) / [ORCID](#)
WEB: <https://soumyajyoti.com>

SUMMARY

- Extensive academic research experience in the field of computational material science involving diverse class of materials using state of the art quantum mechanical and multiscale materials modelling.
- 19 published papers, including: Nat. Comm. = 1, Phys. Rev. B-Rapid Comm. = 2 (first author), Phys. Rev. B = 4 (first author), Nat. Sci. Report = 2, JPCM = 1, JPCC = 1; 2 Book chapters, 3 articles under review, 4 articles in preparation. No. of citations = **360+** ([Google Scholar](#)), h-index = **11**.

PROFESSIONAL EXPERIENCE

- APR. 2017 – PRESENT **University of Kiel, Institute of Theoretical Physics and Astrophysics, Kiel, GERMANY**
Postdoctoral Researcher with Prof. Dr. Stefan Heinze
- DEC. 2016 – MAR. 2017 **Uppsala University, Department of Physics & Astronomy, Uppsala, SWEDEN**
Postdoctoral researcher with Prof. Biplab Sanyal & **System Administrator**
- APR. 2012 – NOV. 2016 **Uppsala University, Department of Physics & Astronomy, Uppsala, SWEDEN**
Doctorand with Prof. Biplab Sanyal and Prof. Olle Eriksson & **System Administrator**
- JUL. 2009 – JAN. 2012 **University of Pune, Centre for Modeling and Simulation & Department of Physics, Pune, INDIA. Junior Research Fellow** with Prof. Dilip Kanhere.

EDUCATION

- APR. 2012 – NOV. 2016 **Doctor of Philosophy in PHYSICS & Licentiate of Philosophy in PHYSICS**
Uppsala University, Department of Physics & Astronomy, Uppsala, SWEDEN.
- JULY 2007 – JUNE 2009 **Master of Science in PHYSICS, Department of Physics, Pune University**
Pune, INDIA. HIGHEST GRADE & TOP 5 within the class.
- AUG. 2004 – JULY 2007 **Bachelor of Science (Honors) in PHYSICS, St. Xavier's College, University of Calcutta, Kolkata, INDIA. First Class Honours.**

RESEARCH EXPERIENCE

- KIEL UNIVERSITY • **Predicted sub-10 nanometer size skyrmion** in ultrathin films which is essential for **skyrmion based spintronic devices** using density functional theory and atomistic spin dynamics.
- Showed that **thermal stability of skyrmions due to entropic effects can be strongly affected by external control parameters such as magnetic field and interface composition**
- **Led the simulation work** to explain recent spin-polarized scanning tunneling microscopy experiments confirming **intra-atomic noncollinear magnetism & tunnelling anisotropic magnetoresistance effect** of adatoms on surfaces with a noncollinear magnetic structure e.g., spin spirals, skyrmions or domain walls.
- PHD & UPPSALA UNIVERSITY • Investigated the **influence of defects and impurities** on the properties of various 2D materials (**PhD thesis**)[\[link\]](#).
- **Predicted formation of metallic cluster** at a interface of in-plane 2D heterostructure of graphene and h-BN using *ab initio* molecular dynamics and nudged elastic band method.
- **Exploration and analysis** of electronic transport properties using **Non Equilibrium Green's Function** in 2D materials e.g., graphene, silicene.
- Investigated **functionalization of various 2D materials** using adatoms, molecular magnets, metal clusters, etc. to tune their properties for applications in spintronic devices.
- Demonstrated **prominent gas sensing activity & site selective fluorination** in defected graphene.

- Studied the surface, interface, edge effects, and **excitonic properties** in 2D materials.
 - Investigated **metal-free photochemical (hydro)silylations & transfer-hydrogenations** in graphene.
 - Used **linear response theory** to predict correct **Hubbard U** values for correlated electron metal center in organometallics and further investigated the effect of ligand on it.
-
- JRF
- **Predicted compact islands formation** of adsorbed hydrogen from graphene to *graphane* showing **semi-metal to metal to insulator transition**.
 - Investigated the structure and melting behavior of supported metallic clusters using *ab initio Molecular Dynamics* simulations.
-
- MASTERS
- Studied the effect **Defects in Semiconductor Clusters** using density functional theory (M.Sc project). The thesis can be found here.[\[link\]](#)

COMPUTATIONAL SKILLS

- SOFTWARE
- Experience working with VASP, Quantum ESPRESSO, FLEUR, SIESTA, TranSIESTA, WIEN2k, Yambo, DFTB+, GPAW, Wannier90, Atomistic Spin Dynamics.
 - Expert in code optimization, porting and maintenance on various high performance computing infrastructure.
-
- DEVELOPMENT
- Developer of various **utility codes** for software related to my research activity.
-
- PROGRAMING LANGUAGES
- Proficient in using Fortran, Python, C, Shell Scripts, Mathematica.
 - Familiarity with C, C++, PHP, HTML, CSS, Javascript
-
- SYSTEM ADMINISTRATION
- Porting scientific applications on a range of HPC platforms, EU-INDIA grid, Garuda grid. Setting up 'Rocks' based HPC cluster for research. **HPC Administration & Linux System Administration**. Designing & maintaining different web servers.
 - Involved in managing, purchasing of computer software & hardware and maintaining network infrastructure, web & storage servers of Materials Theory Division, Uppsala University.

PROFESSIONAL ACTIVITIES

- ORGANIZATION
- Member of organising committee, NU-MATHIMO workshop in Uppsala (June 2015)
 - Project management, writing grants for computer time allocation.
- SUPERVISION
- **Diploma students:** M. Gutzeit (2018), L. Stühmer-Herrmann (2019).
- TEACHING
- Central University of Rajasthan, Rajasthan, India
Computational Physics for undergraduate students. (Visiting lecturer 2012)
- CONFERENCES
- Regular participant of International conferences and workshops. Contributed talks in recent conferences – DPG2019 [\[link\]](#), JEMS2018, SolSkymag2018, DPG2018 [\[link\]](#). Poster presentation in conferences – SPSTM-7, DPG2016 [\[link\]](#)

GRANTS, HONOURS AND AWARDS

- TRAVEL GRANTS
- Graduate school on Advanced Materials travel grant *Sept 2013*
- AWARDS
- Junior Research Fellowship, Indo-Swiss joint research program. *July 2009*
 - National Eligibility Test for Junior Research Fellowship and Lectureship conducted by CSIR and UGC in India *June 2009*

VOLUNTEER EXPERIENCE

- 2014 – 2016
- PhD Student Representative – Equal Opportunity board, Physics dept, Uppsala University.
Responsible for maintaining the interests of PhD students in the ongoing equality work and plans at the department
- 2014 – 2015
- Information Officer – TNDR Board (The PhD students' council of the faculty of science and technology, Uppsala University)
Responsible for maintaining and developing information infrastructure, both physical and virtual
- 2014 – 2015
- Election Committee Member – TNDR
Responsible for conducting and monitoring the election process of TNDR board members and representatives
- 2016
- Student Ambassador – Campus1477 Gym, Uppsala
Responsible for promoting activities of Campus1477 among the Uppsala University students