Soumyajyoti Haldar, PhD

Résumé

Contact Information

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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.
- 21 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 = **390+** (Google Scholar), h-index = **11**.
- Experience in System administration for HPC Linux cluster, servers, Mac OS based systems.

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.
- **Led the theoretical calculations** in a joint theory-experimental work which provides the **first characterization of the exchange force field together with the spin polarization of a spin spiral** & opens the perspective of quantifying different exchange mechanisms of chiral magnetic structures with atomic-scale precision.

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 softwares related to my research activity.

Programing Languages
- Proficient in using Fortran, Python, 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], SPS19 [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.

2014 – 2015 Information Officer – TNDR Board (The PhD students' council of the faculty of science and technology, Uppsala University) & Election Committee Member - TNDR.

2016 Student Ambassador – Campus1477 Gym, Uppsala