

CONTACT INFORMATION

Institute of Theoretical Physics and Astrophysics
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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.
- 18 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 = 350+ ([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.
PhD Thesis: "Influence of impurities and defects on the properties of 2D materials" [\[link\]](#)
Lic. Thesis: "Fe Adatoms on 2D Surfaces: Influence of Defects and Interfaces" [\[link\]](#)
Advisers: Dr. Biplab SANYAL & Prof. Olle ERIKSSON
- JULY 2007 — JUNE 2009 **Master of Science in PHYSICS, Department of Physics, Pune University**
Pune, INDIA. HIGHEST GRADE & TOP 5 within the class.
Major: Condensed Matter Physics
Thesis: "Simulation Studies of Defect in Semiconductor Clusters" [\[link\]](#)
Adviser: Prof. Anjali KSHIRSAGAR
- AUG. 2004 — JULY 2007 **Bachelor of Science (Honors) in PHYSICS, St. Xavier's College, University of Calcutta, Kolkata, INDIA.** First Class Honours.

RESEARCH ACTIVITY

- Broad • In the field of Theoretical and Computational Materials Physics and Chemistry.
 • Materials Modeling for Spintronics and Device Applications through cutting edge computational methodology.
- Specific • Small size skyrmion prediction in ultra-thin film systems.
 • Atomistic spin dynamics applied to complex magnetic systems.
 • Noncollinear magnetic surfaces e.g. Spin spirals
 • Adatoms, dimers, molecular magnets on surfaces.
 • Impurities and defects in various 2D materials.
 • Electronic transport, Gas sensing activities, edge effects, functionalization of 2D materials.

- Cluster-surface interactions using *Ab-initio* Molecular Dynamics simulations.

COMPUTATIONAL SKILLS

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| SOFTWARE | <ul style="list-style-type: none"> • 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. |
| PROGRAMMING LANGUAGES | <ul style="list-style-type: none"> • Proficient in using Fortran, Python, C, Shell Scripts, Mathematica. • Familiarity with C, C++, PHP, HTML, CSS, Javascript |
| SYSTEM ADMINISTRATION | <ul style="list-style-type: none"> • Porting scientific applications on a range of HPC platforms, EU-INDIA grid, Garuda grid. |
| | Setting up 'Rocks' based HPC cluster for research. HPC Administration and Linux System Administration. Designing and maintaining different web servers. |

PROFESSIONAL ACTIVITIES

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| ORGANIZATION | <ul style="list-style-type: none"> • Member of organising committee, NU-MATHIMO workshop in Uppsala (June 2015) • Project management, writing grants for computer time allocation. |
| SUPERVISION | <ul style="list-style-type: none"> • Diploma students: M. Gutzeit (2018), L. Stühmer-Herrmann (2019). |
| TEACHING | <ul style="list-style-type: none"> • Central University of Rajasthan, Rajasthan, India • Computational Physics for undergraduate students. (Visiting lecturer 2012) |
| CONFERENCES | <ul style="list-style-type: none"> • 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

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| TRAVEL GRANTS | <ul style="list-style-type: none"> • Graduate school on Advanced Materials travel grant | Sept 2013 |
| | COMO Summerschool at Lake Como School of Advanced Studies, Como | |
| AWARDS | <ul style="list-style-type: none"> • Junior Research Fellowship | July 2009 |
| | From Indo-Swiss centre to work in a joint Indo-Swiss Research Program | |
| | <ul style="list-style-type: none"> • National Eligibility Test for Junior Research Fellowship and Lectureship conducted by CSIR and UGC in India | June 2009 |
| | For Lectureship qualifications, University Grants Commission, India | |

VOLUNTEER EXPERIENCE

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| 2014 – 2016 | PhD Student Representative – Equal Opportunity board, Uppsala University. Responsible for maintaining the interests of PhD students in the ongoing equality work and plans at the department level |
| 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 |