

## CONTACT INFORMATION

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## SUMMARY

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- 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

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- 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

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- 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

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- 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"> <li>• Experience working with VASP, Quantum ESPRESSO, FLEUR, SIESTA, TranSIESTA, WIEN2k, Yambo, DFTB+, GPAW, Wannier90, Atomistic Spin Dynamics.</li> <li>• Expert in code optimization, porting and maintenance on various high performance computing infrastructure.</li> </ul>
PROGRAMMING LANGUAGES	<ul style="list-style-type: none"> <li>• Proficient in using Fortran, Python, C, Shell Scripts, Mathematica.</li> <li>• Familiarity with C, C++, PHP, HTML, CSS, Javascript</li> </ul>
SYSTEM ADMINISTRATION	<ul style="list-style-type: none"> <li>• Porting scientific applications on a range of HPC platforms, EU-INDIA grid, Garuda grid.</li> </ul> <p>Setting up 'Rocks' based HPC cluster for research. HPC Administration and Linux System Administration. Designing and maintaining different web servers.</p>

## PROFESSIONAL ACTIVITIES

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ORGANIZATION	<ul style="list-style-type: none"> <li>• Member of organising committee, NU-MATHIMO workshop in Uppsala (June 2015)</li> <li>• Project management, writing grants for computer time allocation.</li> </ul>
SUPERVISION	<ul style="list-style-type: none"> <li>• <b>Diploma students:</b> M. Gutzeit (2018), L. Stühmer-Herrmann (2019).</li> </ul>
TEACHING	<ul style="list-style-type: none"> <li>• Central University of Rajasthan, Rajasthan, India</li> </ul> <p>Computational Physics for undergraduate students. (Visiting lecturer 2012)</p>
CONFERENCES	<ul style="list-style-type: none"> <li>• Regular participant of International conferences and workshops. Contributed talks in recent conferences – DPG2019 <a href="#">[link]</a>, JEMS2018, SolSkymag2018, DPG2018 <a href="#">[link]</a>. Poster presentation in conferences – SPSTM-7, DPG2016 <a href="#">[link]</a></li> </ul>

## GRANTS, HONOURS AND AWARDS

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

## 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