DR. SUMANTA BHANDARY

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Personal statement

I am a theoretical condensed matter physicist, specialised in first-principles and many-body theory modelling of bulk and nano-structured materials. My research focuses on numerical method developments in the field of correlated electron systems and multi-level simulations to understand how intricate correlation-induced features emerge in low-dimensional systems. I have an extensive network of collaborations with different experimental groups, particularly specialised in X-ray absorption spectroscopy (including. XMCD), Scanning Tunnelling Microscopy, Photoemission spectroscopy and transport measurements. With these co-operations, in addition to an intrinsic and unwavering curiosity, I strive to identify novel technology-viable materials and mechanisms based on a comprehensive understanding of quantum phenomena.

Current Position

February 2020 – present: Research fellow at School of Physics and CRANN Institute, Trinity College Dublin.

Microscopic origin of emergent magnetism at the organic/molecular-inorganic hetero-interfaces for an economic, environment-friendly alternative for magnetic and spintronic materials.

Previous Appointments

June 2017 – December 2019: Post doctoral researcher at CPHT, Ecole Polytechnique, Palaiseau, France.

Development of multi-level theoretical model of quantum transport in molecular nano-spintronic devices. Theory-experiment cooperation to study the electrode-molecule contact dynamics and its impact on the transport characteristics in molecular nanojunctions.

September 2014 – April 2017: Post doctoral researcher at the Institute for Solid State Physics, TU Wien, Austria.

Development of numerical methods in the field of strongly correlated electron systems: the full charge self-consistent and self-energy self-consistent approaches within combined Density Functional Theory and Dynamical Mean Field Theory (DFT+DMFT) techniques.

Education

Ph.D. [2009 – 2014]: Completed my thesis, entitled "First Principles Studies of Functional Materials Based on Graphene and Organometallics" at the Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden. My thesis advisors were Prof. Biplab Sanyal and Prof. Olle Eriksson.

M.Sc. in Physics [2006 – 2008]: Graduated from the Indian Institute of Technology Guwahati, Assam, India in Physics with **CPA 8.34/10**. I wrote my master's thesis on "Pseudopotentials in Condensed Matter Calculations" under the supervision of Prof. Subhradip Ghosh.

B.Sc. in Physics [2003 – 2006]: Obtained my bachelor's degree with **First-Class Honours** in Physics (major) and Chemistry and Mathematics from the University of Calcutta, Kolkata, India.

Research Interests and Expertise

Strongly correlated electron systems: Developed (Fortran & Python based) 1) charge self-consistency in DFT+DMFT (WIEN2k, Wannier90 and w2dynamics), 2) self-energy self-consistent DFT+DMFT (WIEN2k, Wannier90 and w2dynamics) and 3) Interface for impurity solvers (Exact diagonalization and continuous-time quantum Monte Carlo (CTQMC)) from VASP and Wannier90. I am particularly interested in correlation effects in transition metal-oxides, and in their nano- and hetero-structures.

Molecular electronics and spintronics: Theoretical description of single molecule devices based on magnetic molecules. Multi-level theoretical method development for quantum transport in (correlated) molecular junctions, combining first-principles and many-body theory approaches.

Unconventional magnetism: Tuning magnetic anisotropy (MA) in multilayers; Emergent magnetism in hetero-interfaces. Spinterfaces. Developed code for calculation of MA from second order perturbation theory, interfaced with VASP.

Band-gap engineering in novel 2D materials: Graphene, graphene nano-ribbons, and their chemically functionalised and structurally reconstructed derivatives; role of defects and molecular adsorption.

Teaching Experience

- Tutor for undergraduate course on Thermodynamics at Trinity College Dublin (2021).
- Taught laboratory courses for bachelor studies on Quantum Physics at Uppsala University for two consecutive years (2011 and 2012). The duties included a lecture explaining the details of each experiments, guiding students during the experiment and correcting their laboratory reports.
- Mentoring two final-year undergraduate theses (2021) and supervised a summer student (2021) at Trinity College Dublin (2021).
- During my postdoctoral tenure at CPHT, Ecole Polytechnique, mentored a significant part of a PhD thesis.
- Co-supervised the master's thesis entitled 'Ab initio DFT study of chemically modified graphene' (2009) by Alexander Dochter at Uppsala University.

Research grants

- Småland Nation Ph.D. travel grant 2013.
- Graduate School in Advanced Materials for the 21st Century (GradSAM21) travel grant, December 2012. Scientific collaboration with Prof. Dilip Kanhere at University of Pune, India.
- Graduate School in Advanced Materials for the 21st Century (GradSAM21) travel grant, December 2011. Scientific collaboration with Prof. Indra Dasgupta at Indian Association for Cultivation of Science (IACS), Kolkata, India.

Academic Honors

Prized postdoctoral fellowship in quantum science and technology at the Institut Quantique (IQ), Université de Sherbrooke (2017)[not availed].
PhD fellowship awarded (**qualified in top 1%**) through UGC-CSIR National Eligibility Test (2008).
PhD fellowship awarded (**ranked in top 3%**) through Graduate Aptitude Test for Engineering (2008).
Qualified for Masters program (**ranked in top 4%**) through Joint Admission Test for Masters (2006).

Other trainings

- "Communications, Education and Public Engagement training", AMBER centre, Dublin.
- "Learning to Teach Online", UNSW Sydney.

Invited Talks

- *Correlated molecules for electronics & spintronics: an ab-initio approach*, **IEMN-Lille**, France, November 2019.
- *Organometallic complexes for molecular spintronic devices*, **Lund University**, Sweden, February 2019.
- *Charge self-consistency in DFT+DMFT and beyond*, **Universite de Sherbrooke**, Canada, February 2017.
- *Bistability in magnetic molecules,* **Nu-MATHIMO**, Uppsala, Sweden, June 2015.

- *Organometallics on surfaces: Magnetic anisotropy and Spin dipole,* **University of Bremen**, Bremen, Germany, May 2013.
- *Large magnetocrystalline anisotropy in W_xRe_{1-x}/Fe multilayer,* **ICAM-2011**, Coimbatore, India, December 2011.
- *Graphene as reversible spin manipulator of molecular magnets,* **Complex magnetism in advanced materials**, Duisburg, Germany, September 2011.

Contributed Talks

- *Current manipulation via spin-state switching in magnetic porphyrin connected to graphene electrodes*, **EUROMAT** (virtual), 2021.
- *Effects of electronic correlations on the magnetic properties of organometallic molecules*, **DPG**, Berlin, Germany, March 2018
- *Charge self-consistency in DFT+DMFT with maximally localised Wannier functions: k-space reoccupation and orbital order*, **NGSCES**, Trieste, Italy, September 2016.
- *Electron correlation at the interface : A charge self-consistent DFT+DMFT approach*, **DPG**, Berlin, Germany, March 2015.
- *Manipulating molecule surface magnetic interaction via graphene*, **Magfum V**, Balaton, Hungary, April 2013.
- *Manipulating molecule surface interaction via graphene*, **APS March Meeting**, Baltimore, USA, March 2013.
- *Tuning molecule-surface interaction via graphene*, **Indo-European meeting**, Uppsala, Sweden, June 2012.
- *Manipulating molecule surface exchange interaction via graphene*, **Swedish Graphene Initiative Kick-off Symposium**, Gothenberg, Sweden, December 2011.
- *Large magnetocrystalline anisotropy in $W_{1-x}Re_x$/Fe multilayer*, **Magfum III**, Sovata, Romania, June 2011.
- *Tuning molecular properties by strained defected graphene*, **Indo-European meeting**, Bangalore, India, January 2011.
- *The edge effect*, **Magfum II**, Budapest, Hungary, November 2010.
- *Graphene nano-ribbons from ab-initio theory*, **Frontiers in theoretical magnetism,** Uppsala, October 2009.

Reviewing for international journals

Physics Letters A, Scientific Reports, Physica B, The Journal of Physical Chemistry, Physical Chemistry Chemical Physics.

Publications [Google scholar link]

- J. M. Shaw, R. Knut, C.J. Armstrong, **S. Bhandary**, Y. Kvashnin, Danny Thonig, E. K. Delczeg-Czirjak, O. Karis, T.J. Silva, E. Weschke, H. T. Nembach, O. Eriksson, D. Arena, *Quantifying spin-mixed states in ferromagnets*, Phys. Rev. Lett. **127**, 207201 (2021).
- **S. Bhandary**, S. Haldar, and B. Sanyal *Quasiperiodic van der Waals heterostructures of graphene and hexagonal boron nitride*, Physica Status Solidi B, 2100423 (2021).
- **S. Bhandary**, J. M. Tomczak, A. Valli, *Designing a mechanically driven spin-crossover molecular switch via organic embedding*, Nanoscale Adv., *3*, 4990-4995 (2021).
- **S. Bhandary**, Karsten Held, *Self-energy self-consistent density functional theory plus dynamical mean field theory*, Phys. Rev. B *103*, 245116 (2021).

- D. Schmitz, C. Schmitz-Antoniak, F. Radu, H. Ryll, C. Luo, **S. Bhandary**, S. Biermann, K. Siemensmeyer, H. Wende, S. Ivanov, O. Eriksson *Soft X-Ray Magnetic Circular Dichroism of Vanadium in the Metal-Insulator Two-Phase Region of Paramagnetic V2O3 Doped with 1.1% Chromium*; Phys. Status Solidi B, *257*, 1900456 (2020).
- J. Steinbauer, S. Biermann, **S. Bhandary** *Role of charge transfer in hybridization-induced spin transition in metal-organic molecules*; Phys. Rev. B *100*, 245418 (2019).
- R. H. Kou, J. Gao, Y. Ren, B. Sanyal, **S. Bhandary**, S. M. Heald, F. Brandon, C. -J. Sun *Charge transfer-tuned magnetism in Nd-substituted* Gd_5Si_4; AIP Advances *8 (12)*, 125219 (2018).
- S. Haldar, **S. Bhandary**, H. Vovusha, and B. Sanyal *Comparative study of electronic and magnetic properties of iron and cobalt phthalocyanine molecules physisorbed on two- dimensional* MoS_2 *and graphene*; Phys. Rev. B *98*, 085440, (2018).
- C. Schmitz-Antoniak, D. Schmitz, A. Warland, M. Darbandi, S. Haldar, **S. Bhandary**, B. Sanyal, O. Eriksson, H. Wende *Suppression of the Verwey Transition by Charge Trapping*; Ann. Phys.(Berlin), 530, 1700363, (2018).
- **S. Bhandary**, E. Assmann, M. Aichhorn, K. Held *Charge self-consistency in density functional theory + dynamical mean field theory:* **k***-space reoccupation and orbital order*; Phys. Rev. B *94*, 155131, (2016).
- **S. Bhandary**, M. Schüler, P. Thunström, I. di Marco, B. Brena, O. Eriksson, T. Wehling, and B. Sanyal. *Correlated electron behavior of metal-organic molecules: Insights from density functional theory combined with many-body effects using exact diagonalization*; Phys. Rev. B *93*, 155158, (2016).
- M. Nordlund, **S. Bhandary**, B. Sanyal, N. Almqvist, T. Löfqvist, H. Grennberg *Side-selective self-assembly of graphene and FLG on piezoelectric PVDF from suspension*; J. Phys. D: Applied Physics*49(7)*, 07LT01, (2016).
- **S. Bhandary**, G. Penazzi, J. Fransson, T. Frauenheim, O. Eriksson, B. Sanyal. *Controlling Electronic Structure and Transport Properties of Zigzag Graphene Nanoribbons by Edge Functionalization with Fluorine*; J. Phys. Chem. C *119(36)*, 21227, (2015).
- D. Schmitz, C. Schmitz-Antoniak, A. Warland, M. Darbandi, S.Haldar, **S. Bhandary**, O. Eriksson, B. Sanyal, and H. Wende. *The dipole moment of the spin density as local indicator for phase transitions*; Nat. Sci. Rep. *4*, 5760, (2014).
- S. Haldar, B. S. Pujari, **S. Bhandary**, F. Cossu, O. Eriksson, D. G. Kanhere, B. Sanyal. *Fe*$_n$ *clusters (*n*=1-6) chemisorbed on vacancy defects in graphene: Stability, spin-dipole moment and magnetic anisotropy*; Phys. Rev. B *89*, 205411, (2014).
- D. Klar, **S. Bhandary**, A. Candini, L. Joly, P. Ohresser, S. Klyatskaya, M. Ruben, M. Affronte, O. Eriksson, B. Sanyal, and H. Wende. *Field-regulated switching of the magnetization of Co-porphyrin on graphene*; Phys. Rev. B *89*, 144411, (2014).
- H. C. Herper, **S. Bhandary**, O. Eriksson, B. Sanyal, and B. Brena. *Fe phthalocyanine on Co(001): Influence of surface oxidation on structural and electronic properties.*; Phys. Rev. B *89*, 085411, (2014).
- D. Klar, B. Brena, H. C. Herper, **S. Bhandary**, C. Weis, B. Krumme, C. Schmitz-Antoniak, B. Sanyal, O. Eriksson, H. Wende. *Oxygen-tuned magnetic coupling of Fe-pthalocyanine molecules to ferromagnetic Co films.*; Phys. Rev. B *88*, 224424, (2013).
- **S. Bhandary**, O. Eriksson, B. Sanyal. *Defect controlled magnetism in FeP/graphene/Ni(111)*; Nat. Sci. Rep. *3*, 3405, (2013).
- H. C. Harper, M. Bernie, **S. Bhandary**, C. F. Hermanns, A Kruger, J. Miguel, C. Weis, C. Schmitz-Antoniak, B. Krumme, D. B. Chen, C. Tieg, B. Sanyal, E. Weschke, C. Czekelius, W. Kuch, H. Wende, O. Eriksson. *Iron porphyrin molecules on Cu (001): Influence of adlayers and ligands on the magnetic properties*; Phys. Rev. B *87*, 174425, (2013).
- **S. Bhandary**, B. Brena, P. M. Panchmatia, I. Brumboiu, M. Bernien, C. Weis, B. Krumme, C. Etz, W. Kuch, H. Wende, O. Eriksson, B. Sanyal. *Manipulation of spin state of iron porphyrin by chemisorption on magnetic substrates*; Phys. Rev. B *88*, 024401, (2013).

- Y Hajati, T. Blom, S. H. M. Jafri, S. Haldar, **S. Bhandary**, M. Z. Shoushtari, O. Eriksson, B. Sanyal, K. Leifer. *Improved gas sensing activity in structurally defected bilayer graphene*; Nanotechnology *23*, 505501, (2012).
- S. Haldar, **S. Bhandary**, S. Bhattacharjee, O. Eriksson, D. Kanhere, B. Sanyal. *Functionalization of edge reconstructed graphene nanoribbons by H and Fe: A density functional study*; Solid State Comm. *152*, 1719724, (2012).
- B. Dutta, **S. Bhandary**, S. Ghosh and B. Sanyal. *A first principles study of magnetism in Pd_3Fe under pressure*; Phys. Rev. B *86*, 024419, (2012).
- **S. Bhandary**, S. Ghosh, H. Herper, H. Wende, O. Eriksson and B. Sanyal. *Graphene as a reversible spin manipulator of molecular magnets*; Phys. Rev. Lett. *107*, 257202, (2011).
- E. Holmström, J. fransson, O. Eriksson, R. Lizarraga, B. Sanyal. **S. Bhandary** and M. I. Katsnelson. *Disorder-induced metallicity in amorphous graphene*; Phys. Rev. B *84*, 205414, (2011).
- **S. Bhandary**, O. Granäs, L. Szunyogh, B. Sanyal , L. Nordström and O. Eriksson. *Route towards finding large magnetic anisotropy in nanocomposites: application to a $W_{1-x}Re_x/Fe$ multilayer*; Phys. Rev. B *84*, 092401, (2011).
- J. Zhu, **S. Bhandary**, B. Sanyal and H. Ottoson. *Interpolation of atomically thin hexagonal boron nitride and graphene: electronic structure and thermodynamic stability in terms of all-carbon conjugated paths and aromatic hexagons*; J. Phys. Chem. C *115(20)*, 10264, (2011).
- J. M. Wikeberg, R. Knut, **S. Bhandary**, I. DiMarco, M. Ottoson, J. Sadowski, B. Sanyal, P. Palmgren, C. W. Tai, O. Eriksson, O. Karis, P. Svedlindh . *Magnetocrystalline anisotropy and uniaxiality of MnAs/GaAs(100) films*; Phys. Rev. B *83*, 024417, (2011).
- **S. Bhandary**, M. I. Katsnelson, O. Eriksson and B. Sanyal. *Complex edge effects in zigzag graphene nanoribbons due to hydrogen loading*; Phys. Rev. B *82*, 165405, (2010).

Book Chapters

- H. C Herper, B. Brena, C. Puglia, **S. Bhandary**, H. Wende, O. Eriksson, B. Sanyal, *Molecular Nanomagnets: Fundamental Understanding* Springer, Singapore (2020).
- H. C. Herper, B. Brena, **S. Bhandary** and B. Sanyal, *Deposited Transition Metal-Centered Porphyrin and Phthalocyanine Molecules: Influence of the Substrates on the Magnetic Properties*, InTechOpen (2017).
- **S. Bhandary** and B. Sanyal. *Graphene-boron nitride composite: a material with advanced functionalities*; InTechOpen (2012).
- S. Haldar, **S. Bhandary**, P. Chandrachud, B. Pujari, M. I. Katsnelson, O. Eriksson, D. G. Kanhere, B. Sanyal. *Ab Initio Studies on the Hydrogenation at the Edges and Bulk of Graphene*, Graphita 2011, Springer berlin heidelberg (2012).

Languages: English *(full professional proficiency)*, Bengali *(first-language)*, Hindi *(proficient)*.

Interests

Passionate Photographer. Check out some of my recent works here. Out-door sports: *Cricket*: Represented Vienna Cricket Club in Austrian cricket league. Represented Uppsala Internationals and Uppsala Cricket Förening in Swedish Cricket League. *Indoor sports:* Badminton, Table tennis. Organizing social events: Former management member of Uppsala Indian Community.

References

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