Shishir Kumar PANDEY

Curriculum Vitæ

International Academic City, P.O. No.-345055, Dubai, UAE
+971-507890589
shishir.kr.pandey@gmail.com, shishir@dubai.bits-pilani.ac.in
https://sites.google.com/site/shishirkrpandey
Shishir Kumar Pandey
shishirkpandey

Live as if you were to die tomorrow,
Learn as if you were to live forever. ∼ Mahatma Gandhi

Personal details

Date of birth: **20/04/1988**
Nationality: **Indian**
Gender: **Male**

Current Position

May 2024– **Assistant Professor**, *BITS-Pilani, Dubai Campus, UAE*, Dept. of General Sciences

Education and Academic degrees

2011–2018 **Ph.D.**, *Dept. of Condensed Matter Physics and Material Science*, S. N. Bose National Center for Basic Sceinces, Kolkata, India
Title *Microscopic Model for Spin, Charge and Orbital ordering in Transition Metal Compounds*
Supervisor Prof. Priya Mahadevan, S. N. Bose National Center for Basic Sceinces, Kolkata, India
2009–2011 **M.Sc.**, *in Applied Physics*, ISM (Indian Institute of Technology [IIT]) Dhanbad, India
2009 **B.Sc.**, *With Physics, chemistry and mathematics*, Ewing Christian College, University of Allahabad, India

Research Experience

AI for Science Institute, Beijing, China

Jan 2022–Feb 2024 **Understanding fundamental aspects of materials properties using machine learning, particularly across various phase transitions.**,
Research Scientist

International Center for Quantum Materials, Peking University, Beijing, China

Jan 2019–Dec 2021 **Magnetic and superconducting properties of transition metal compounds**,
Post-doctoral fellow,
Mentor : Prof. Ji Feng,
Investigated the magnetic and supercondcting properties of $3d$ and $4d$ transition metal compounds of pertinent quantum spin-liquid candidates and cuprate analogues using combination of first-principle methods, model Hamiltonian approach and linear response techniques.

Dept. of Physics, National Taiwan University, Taiwan

June 2018–Dec 2018 **Structural phase transitions in Hg-based perovskites**,
Research Associate,
Mentor : Prof. Guan-Yu Guo,
First-principle based investigation of structural transitions in Hg-based perovskites oxides.

Dept. of Condensed Matter Physics, Institute of Physics, Bhubaneshwar, India

Jan 2018–March 2018 **Electronic properties of hybrid perovskite material**,
Visiting Scholar,
Mentor : Prof. Saptarshi Mandal,
In collaboration with experimental group of Prof. Dinesh Topwal, first-principle based study to understand the role of orintational disorder of organic molecule on electronic structure in a hybrid perovskite material.

S. N. Bose National Center for Basic Sciences, Kolkata, India

Oct 2011–Sep. 2017 **Microscopic Model for Spin, Charge and Orbital ordering in Transition Metal Compounds**, *Ph.D fellow*,
Mentor : Prof. Priya Mahadevan,
We studied magnetic and electronic properties of perovskite bulk as well as 2D transition metal dichalcogenides using a combination of first-principle method, model Hamiltonian approach and statistical simulation method like Monte Carlo technique.

Research Interests

Weakly and strongly correlated Systems, many-body models

I focus on applying and developing computational physics apparatuses to study the electronic structure and physical properties of condensed matter systems. I do so by harnessing the power of accurate first-principles electronic structure methods and a number of theoretical tools. Materials of interest include both the weakly as well as the strongly correlated systems and the computational tool involve $ab\ initio$ techniques, linear response methods, model Hamiltonian-based analytical/numerical approaches, renormalization group based method and statistical simulation method. Through my studies, I have indulge myself in obtaining a comprehensive understanding of materials behavior and utilize it to suggest new routes to realize exotic quantum phases of matter. Some of the physical phenomena I am currently focusing on includes realization of quantum spin-liquid state in so-called spin-orbit assisted Mott insulators, magnetic quantum phase diagrams for magnetic materials with experimentally tunable parameters, charge and spin density wave transitions in quasi- 1D and 2D materials. I have an eager to extend the horizon of my computational skills. So, my current focus of research is on deep learning based modeling of materials with strong magnetoelastic coupling and coupled magnetic-structural phase transitions. The outcome of my research is of interest to both theoretical and experimental research community.

Computational skills

$Ab\ initio$ modeling tools: **DFT and TB packages**, Plane wave based methods-Vienna ab-initio Simulation Package (VASP) and Quantum Espresso, Linearized Augmented Planewave (LAPW) Method as implemented in Wien2k codes, Full-potential local-orbital method as implemented in FPLO, Open source package for Material eXplorer (OpenMX); AIMD; Wannier90 code; WannierTools

Packages: **Miscellaneous**, Mathematica, MATLAB, Phonopy, ICET (cluster expansion), SpinW (Linear spin-wave spectra), pymatgen, SpinParser (pseudo-fermion renormalization group calculations), LAMMPS (Molecular dynamics), PyTorch

Code development: **Many-body, linear response and Monte Carlo codes**, Mean-field study-Hartree-Fock approximation, Multiorbital Hubbard-Kanamori model to use in second-order perturbation method, cRPA and FLEX codes to understand charge and spin instability driven phase transitions (detection of CDW and superconducting behavior), code to extract spin-orbit coupling strength from $ab\ initio$ band structure, Monte Carlo codes to simulate magnetic properties, parts of DeepTB (A deep potential-based TB model)

Programming: **Coding languages**, Fortran90; Python3; Shell scripting, Latex

Collaborative experience

Experimental

Prof. Dinesh Topwal, at IOP, Bhubaneshwar

Prof. Mintu Mandal, at IACS, Kolkata

Dr. Soumya Jyoti Ray, at IIT, Patna

Dr. Pankaj R Sagdeo, at IIT, Indore

Theoretical

Dr. Rajarshi Tiwari, at Trinity College, Dublin

Prof. Ashis K. Nandy, at NISER, Bhubaneshwar

Dr. Stephen M. Winter, at Wake Forest University, NC, USA

Dr. Oleksandr Malyi, at ENSEMBLE3, Warsaw, Poland

Mentoring experience

Dr. Qiangqiang Gu, School of Mathematics, Peking University
Title: Investigation of a designing route for new Quantum spin-liquid candidates (June 2022–Feb 2024)

Undergraduate students

Krish Bharat Khatri, Yuvaraj Jagadish Nayak at BITS-Dubai
Title: Study of anhormonicity in crystalline solids at finite temperatures using Deep-potential models (Jan-Jun 2025)

Jessica Hanna Thomas, Md. Affaan Sayed, Purab Rihal, Venkata Shreya Vella at BITS-Dubai
Title: Spintronics Driven ML-Assisted Neuromorphic Computation (Jan-Jun 2025)

Fellowships & Recognitions

2024: **Ramanujan Fellowship by SERB, India**, *at IIT, Jammu*
2016: **Graduate Aptitude Test in Engineering (GATE)**, *Qualified an All India level exam*
2015: **Best oral presentation award**, *Bose Fest 2015*, at SNBNCBS, Kolkata
2012: **CSIR-UGC NET**, *for PhD from All India National Eligibility Test*
2011: **Overall third position**, *in M.Sc. batch of 2009*
2010: **Merit cum mean stipend**, *from ISM (IIT), Dhanbad*

Professional services

Referee of Phys. Rev. Lett., Phys. Rev. B, PCCP, Bulletin of Materials Science (BOMS, Springer Nature) etc

Invited Talk

Dec 2023 **"Computational exploration of a viable route to Kitaev-quantum spin liquid phase in $OsCl_3$"**, Guangdong University of Technology, China

Jan 2022 **"Experimental signature of Quantum Spin-liquid phase in materials"**, at AI for Science Institute, Beijing

Sep 2019 **"Doping an antiferromagnetic insulator: A route to an antiferromagnetic metallic phase"**, at Peter Grunberg Institute (PGI), Germany

Contributed talks, conferences and schools

Sep 2019 **"Doping an antiferromagnetic insulator: A route to an antiferromagnetic metallic phase"**, *talk delivered*, at Peter Grunberg Institute (PGI), Germany

Sep 2019 **"Correlated Electrons: Many body methods for Real Materials"**, *autumn School attended*, at Forschungszentrum, Julich

Dec 2018 **"Recent Developments in Chiral Matter and Topology"**, *workshop attended* , at National Taiwan University, Taipe

June 2018 **"The 16th Workshop on FirstPrinciples Computational Materials Physics"**, *workshop attended*, at National Tsing-Hua University, Hsinchu, Taiwan

Feb 2018 **"Annual Condensed Matter Physics Meeting"**, *talk delivered*, at NISER, Bhubaneshwar,
titled: Doping an antiferromagnetic insulator: A route to an antiferromagnetic metallic phase

Jan 2017 **"Indo-US Bilateral Workshop On Physics and Chemistry of Oxides: Theory meets experiments"**, *presented poster*, at SNBNCBS, Kolkata

Jan 2016 **"Emerging Trends in Advanced Functional Materials"**, *talk delivered*, at IOP, Bhubaneswar

Dec 2015 **"XXVII IUPAP Conference on Computational Physics"**, *contributory talk delivered*, at IIT, Guwahati

Aug 2014 **"CMDAYS-14"**, *presented poster*, at Calcutta University

Feb 2014 **"Advanced Functional Magnetic Materials"**, *DST-SERC School attended* , at Goa University

Dec 2013 **"International Conference on Directions in Materials Science"**, *presented poster* , at JNCASR, Bangalore

Feb 2013 **"Quantum Monte Carlo Electronic Structure Calculation"**, *JAIST International Winter School attended* , at JAIST, Ishikawa, Japan

Apr 2012 **"ATHENA-2012"**, *international school attended* , at SNBNCBS, Kolkata

Apr 2011 **"International School/Conference on Functional Materials"**, *international conference attended* , atHarish-Chandra Research Institute, Allahabad, India