Abhilash Patra

PERSONAL DETAILS

. *Work*	Postdoctoral Scholar
.	Department of Chemistry & Biochemistry
.	University of South Carolina, Columbia, SC, 29208
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. *Scholar*	https://scholar.google.com/citations?user=CDKHI4MAAAAJ&hl=en
. *Researchgate*	https://www.researchgate.net/profile/Abhilash_Patra
. *Github*	https://github.com/abhilash-patra
. *Home Page*	https://sites.google.com/view/abhilashpatra/home?authuser=1

ACADEMICS

Postdoctoral Research Scholar March 1, 2024 - Feb. 28, 2025

Department of Chemistry & Biochemistry,
University of South Carolina, US

Principal Investigator: Dr. Christopher Sutton
project: BEAST, FLOSIC

Postdoctoral Research Scholar Feb 2, 2022 - Feb. 29, 2024.

Mork Family Department of Chemical Engineering and Material Science,
University of Southern California, US

Principal Investigator: Dr. Shaama Mallikarjun Sharda
project: Exascale Computing for Catalytic Design

Ph.D., Physics
"Density Functional Theory" Jan, 2015 - Aug, 2021
School of physical sciences
National Institute of Science Education and Research,
Homi Bhabha National Institute, India

Supervisors: Dr. Prasanjit Samal
Thesis Title: Advance density functionals based on model exchange holes for a wide range of molecular and solid-state systems

M.Sc, Physics 2011-2013
Fakir Mohan University, Balasore, Odisha

National level examinations(India) 2013-2014
CSIR-National Eligible Test, Joint Entrance Screening Test, Graduate Aptitude Test in Engineering (GATE) Physics

RESEARCH INTEREST

My research is based on computationally predicting the electronic structure of atoms, molecules, and bulk solids to clusters. I am interested in the development of density functional theory and higher-order wave function-based methods and their application in contemporary systems. The current focus is the **development of workflow automation to carry out high-throughput studies of excited-state**

systems, implementation of FLOSIC, and Application of MLIP for electronic and optical properties of chiral perovskites.

DFT Development
Development of new exchange-correlation energy functionals
FLO-SIC
New exchange-only potentials
Ab initio molecular dynamics
Hybrid methods
Functionals for dispersion-dominated systems
DFT+U and CRPA methods
TDDFT, Excited state calculation, and RPA
Application of ML in functional development

APLICATIONS OF DFT
Low-dimensional quantum systems
Two-dimensional materials, 2D magnets
Surfaces, interface, and Adsorption
Computational Catalysis and Photochemistry
Study of vibrational and magnetic properties of solids
Multiferroics, Topological Insulators
Application of ML in material discovery and catalysis

TEACHING

Teaching Assistant NISER, India
Atoms, Molecules, and Radiation
Even Sem., 2016

Teaching Assistant NISER, India
Mechanics and Thermodynamics
Odd Sem., 2016

Teaching Assistant NISER, India
Atoms, Molecules, and Radiation
Even Sem. 2017

PUBLICATIONS

1. "The metal-ligand local mode as a descriptor for catalytic activity.", **Abhilash Patra**, Pallavi Sarkar, Shaama Mallikarjun Sharada, Polyhedron **2024**, 267, 117336.

2. "Understanding the Key Factors for Photoinduced Radical Generation in Crystalline Triphenylamines Using Experiment and Machine Learning.", Gamage Isuri P Wijesekera, Fahidat A Gbadamosi, Muhammad Saddam Hossain, **Abhilash Patra**, Christopher Sutton, Linda S Shimizu, *The Journal of Physical Chemistry C*, **2024**, 128, 39, 16713–16720

3. "Performance of Density Functionals for Excited-State Properties of Isolated Chromophores and Exciplexes: Emission Spectra, Solvatochromic Shifts, and Charge-Transfer Character.", **Abhilash Patra**, George Baffour Pipim, Anna I. Krylov, and Shaama Mallikarjun Sharada, *The Journal Chemical Theory and Computation*, **2024** 20, 6, 2520–2537.

4. "Simulating Excited-State Complex Ensembles: Fluorescence and Solvatochromism in Amine-Arene Exciplexes.", **Abhilash Patra**, Anna I. Krylov, and Shaama Mallikarjun Sharada, *The Journal of Chemical Physics*, **2023**, 159, 064101.

5. "Recent Advances toward Efficient Calculation of Higher Nuclear Derivatives in Quantum Chemistry.", Selin Bac, **Abhilash Patra**, Kareesa J. Kron, and Shaama Mallikarjun Sharada, *The Journal of Physical Chemistry A*, **2022**, 126, 43, 7795–7805.

6. "Accurate band gaps from exchange potentials designed from cuspless hydrogen density-based exchange hole model.", **Abhilash Patra**, Bikash Patra and Prasanjit Samal,*Physical Chemistry Chemical Physics*, **2022**, 24, 13633-13640.

7. "Phase evolution in thermally annealed Ni/Bi multilayers studied by X-ray absorption spectroscopy", Bidyadhar Das, Madhusmita Sahoo, **Abhilash Patra**, Ashok K Yadav, SN Jha, Prasanjit Samal, Kartik Senapati, and Pratap K Sahoo, *Physical Chemistry Chemical Physics*, **2022**, 24, 4415-4424.

8. "Band gap of two-dimensional materials: thorough assessment of modern density functional theory methods", Fabien Tran, Peter Blaha, Tomas Rauch, Pedro Borlido, Silvana Botti, Miguel A. L. Marques, **Abhilash Patra**, and Prasanjit Samal. *The Journal of Chemical Physics*, **2021**, 155, 104103.

9. " Efficient band structure calculation of two-dimensional materials from semilocal density functionals", **Abhilash Patra**, Subrata Jana, Prasanjit Samal, Fabien Tran, Leila Kalantari, Jan Doumont, and Peter Blaha. *Journal of Physical Chemistry C*, **2021**, 125 (20), 11206.

10. "Insights from the density functional performance of water and water-solid interactions: SCAN in relation to other meta-GGAs", Subrata Jana, **Abhilash Patra**, Szymon Śmiga, Lucian A. Constantin, and Prasanjit Samal, *The Journal of chemical physics*, **2020**, 153 (21), 214116.

11. " A way of resolving the order-of-limit problem of Tao-Mo semilocal functional", **Abhilash Patra**, Subrata Jana and Prasanjit Samal, *The Journal of chemical physics*, **2020**, 153 (18), 184112.

12. "Electronic band structure of layers within meta generalized gradient approximation of density functionals", **Abhilash Patra**, Bikash Patra, Lucian A. Constantin, and Prasanjit Samal, *Physical Review B*, **2020**, 102 (4), 045135.

13. "Efficient yet Accurate Dispersion-Corrected Semilocal Exchange-Correlation Functionals For Non-Covalent Interactions", **Abhilash Patra**, Subrata Jana, Lucian A. Constantin, and Prasanjit Samal, *The Journal of chemical physics*, **2020**, 153, 084117.

14. "Improved transition metal surface energies from a generalized gradient approximation developed for quasi two-dimensional systems", **Abhilash Patra**, Subrata Jana, Lucian A. Constantin, Letizia Chiodo, and Prasanjit Samal, *The Journal of chemical physics*, **2020**, 152 (15), 151101.

15. "Screened range-separated hybrid by balancing the compact and slowly varying density regimes: Satisfaction of local density linear response", Subrata Jana, **Abhilash Patra**, Lucian A. Constantin, and Prasanjit Samal, *The Journal of chemical physics*, **2020**, 152 (4), 044111.

16. "Adiabatic connection in density functional theory in two-dimensions: A semi-analytic wavefunction based study for two-electron atomic systems", Rabeet Singh, Bikash Patra, **Abhilash Patra**, Manoj K Harbola, and Prasanjit Samal, *The Journal of chemical physics*, **2019**, 151 (20), 204104.

17. "Performance of Tao-Mo Semilocal Functional with rVV10 Dispersion-Correction: Influence of Different Correlation", **Abhilash Patra**, Subrata Jana and Prasanjit Samal, *The Journal of Physical Chemistry A*, **2019**, 123 (49), 10582-10593.

18. "Long-range screened hybrid-functional theory satisfying the local-density linear response",Subrata Jana, **Abhilash Patra**, Lucian A. Constantin, Hemanadhan Myneni and Prasanjit Samal, *Physical Review A*, **2019** 99 (4), 042515.

19. "Colle-Salvetti type correlation functionals for two-dimensional quantum dot systems", **Abhilash Patra** and Prasanjit Samal, *Chemical Physics Letters*, **2019**, 720, 70-75.

20. "Laplacian free and asymptotic corrected semilocal exchange potential applied to the band gap of solids", **Abhilash Patra**, Subrata Jana, Hemanadhan Myneni and Prasanjit Samal, *Physical Chemistry Chemical Physics*, **2019**, 21 (35), 19639-19650.

21. "Efficient lattice constants and energy band gaps for condensed systems from a meta-GGA level screened range-separated hybrid functional", Subrata Jana, **Abhilash Patra** and Prasanjit Samal, *Journal of Chemical Physics*, **2018**, 149, 094105.

22. "Assessing the performance of the Tao-Mo semilocal density functional in the projector-augmented-wave method", Subrata Jana, **Abhilash Patra** and Prasanjit Samal, *Journal of Chemical Physics*, **2018**, 149, 044120.

23. "Inhomogeneity induced and appropriately parameterized semilocal exchange and correlation energy functionals in two-dimensions", **Abhilash Patra**, Subrata Jana and Prasanjit Samal, *The Journal of Chemical Physics*, **2018**, 148, 134117.

24. "A Parameter-Free Semilocal Exchange Energy Functional for Two-Dimensional Quantum Systems", **Abhilash Patra**, Subrata Jana and Prasanjit Samal, *The Journal of Physical Chemistry A*, **2018**, 122(13), 3455-3461.

25. "Gradient approximated exchange energy functionals with improved performances for two-dimensional quantum dot systems", Subrata Jana, **Abhilash Patra** and Prasanjit Samal, *Physica E*, **2018**, 97, 268-276.

UNDER PREPARATION

1. Examining Dynamic Structural Descriptors of Spin-Splitting in 2D Hybrid Perovskites., Abhilash Patra, Nima Karimitari, and Christopher Sutton

2. Application of Machine Learning Interatomic Potential in Exploring Structural Descriptors for Optical Properties of 2D Hybrid Perovskites.

3. Accurate Lithium intercalation potential from density functional theory. Abhilash Patra and Prasanjit Samal

4. Spin-Phonon interaction in quasi 2D-Cr_2Te_3 (Experimental collaboration)

5. "Raman Spectra analysis of Bi and $NiBi_3$ phases in thermally annealed Ni/Bi multilayers" (Experimental collaboration)

CONFERENCE

1. Poster:-"Simulating Excited-State Complex Ensembles: Fluorescence and Solvatochromism in Amine-Arene Exciplexes.", **Abhilash Patra**, TDDFT School and Workshop, Rutgers University, Newark, US, 2023.

2. Talk:- " Workflow Automation in Predicting Exciplex Formation in Arene-Amine complexes", **Abhilash Patra**, 2022 AIChE Annual Meeting, Phoenix Convention Center, Phoenix, AZ, USA.

3. Attended, 7th BerkeleyGW Tutorial Workshop and 2nd Berkeley Excited States Conference (BESC2021), January, 2021.

4. Poster:-"A Colle-Salvetti type correlation functional for two dimensional systems", **Abhilash Patra**, National Conference on Recent Trends in Condensed Matter Physics (RTCMP 2017), Bose Institute, Kolkata, West Bengal-700054, India.

5. Poster:-"An Assessment of Semi-local Exchange potentials in the Band Gap Calculation", **Abhilash Patra**, International Workshop on Advanced Materials (IWAM-2017), National Institute of Science & Technology, Berhampur, Orissa-761008, India.

6. Poster:-"Family of Becke potentials: An assessment in band gap calculations", **Abhilash Patra**, International Workshop on Evolution of Electronic Structure Theory & Experimental Realization (EESTER 2018), SRM Institute of Science and Technology & Indian Institute of Technology Madras, Tamil Nadu-600036, India.

EXPERIENCE IN CODING AND SOFTWARE

Languages
Fortran, Python, Mathematica, Matlab

Functional implementation and calculation
WIEN2k, VASP, NWCHEM, QCHEM, JDFTx, QimPy

Other codes
Exciting, Quantum espresso, GPAW, Octopus, deMon2k, FHI-aims, ADF, Abinit, Yambo, BerkeleyGW, WannierTools, QMCPACK, VAMPIRE, JDFTx, QimPy

Workflow
FireWorks, Custodian, Pymatgen

Useful packages
XCrySDen, Avogadro, Atomic Simulation Environment (ASE), p4vasp, gnuplot, xmgrace, Inkspace, GIMP, VESTA, IQmol

ACADEMIC REFERENCES

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Prof. Shaama M. Sharada
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