

Subrata Jana

School of Physical Sciences

National Institute of Science Education and Research

PO - Bhimpur - Padanpur, Via - Jatni, District - Khurda, PIN-752050, Odisha, INDIA

Phone: +91 9735694106

Fax: +91 (674) 2494262

Email: subrata.jana@niser.ac.in, subrata.niser@gmail.com

Born: October 13, 1989—West Bengal, INDIA

Nationality: Indian

CURRENT POSITION

Research Scholar, School of Physical Sciences, National Institute of Science Education and Research, INDIA

AREAS OF SPECIALIZATION

Density Functional Theory, Theoretical Condensed Matter Physics, Computational Chemistry.

ACADEMICS

2007	UNDERGRADUATE STUDIES West Bengal Council of Higher Secondary Education, West Bengal, INDIA
2010	BACHELOR OF SCIENCE (B.Sc.) in Physics, Vidyasagar University, Midnapur, Wst Bengal, INDIA
2012	MASTER OF SCIENCE (M.Sc.) in Physics, Indian Institute of Engineering Science and Technology, Shibpur, INDIA (Formerly Bengal Engineering and Science University, Shibpur, INDIA)
2013-	PhD (Ongoing) in Theoretical Condensed Matter, National Institute of Science Education and Research, Bhubaneswar, INDIA

RESEARCH INTERESTS:

My research activity is focused on theoretical and computational condensed matter physics, primarily studying the electronic structure of atoms, molecules and solids employing density functional methods. Materials design, including computing electronic, magnetic and structural properties and responses from first principles using density functional theory, and other suitable quantum many-body techniques.

The main research interest at present includes:

- Methodological developments and application of ground state density-Functional
- Development of meta-GGA level range-separated hybrid functional theory and its application to the atoms, molecules and solids
- Development of exchange energy functional for two dimensional quantum systems
- Development of GGA and meta-GGA level functional for time independent excited state density functional theory
- Application of the meta-GGA level semilocal screened hybrid functional in time dependent density functional theory
- Development and application of linear response meta-GGA kernel in solids through the screened meta-GGA level density
- Dielectric dependent range-separated hybrid functional theory
- Development of norm-conserving pseudo-potential for the meta-GGA level semilocal and screened hybrid functional
- van der Waals-corrected Density Functional Theory
- Nanostructures & Properties of Materials
- Beyond density functional theory: GW and Bethe-Salpeter

PUBLICATIONS, TALKS & SEMINERS

JOURNAL ARTICLES

Published

1. Semilocal Exchange Energy Functional for Two-Dimensional Quantum Systems: A Step Beyond Generalized Gradient Approximations, S. **Jana** and P. Samal, J. Phys. Chem. A 121, 4804 (2017). <https://pubs.acs.org/doi/abs/10.1021/acs.jpca.7b03686>
2. Gradient approximated exchange energy functionals with improved performances for two-dimensional quantum dot systems, S. **Jana**, A. Patra and P. Samal, Phys. E 97, 268-276 (2018). <https://doi.org/10.1016/j.physe.2017.11.019>
3. Exploration of near the origin and the asymptotic behaviors of the Kohn-Sham kinetic energy density for two-dimensional quantum dot systems with parabolic confinement, S. **Jana** and P. Samal, J. Chem. Phys. 148, 024111 (2018). <https://doi.org/10.1063/1.5009495>
4. Long-range corrected density functional through the density matrix expansion based semilocal exchange hole, B. Patra, S. **Jana** and P. Samal, Phys. Chem. Chem. Phys., 20, 8991-8998 (2018). <http://dx.doi.org/10.1039/C8CP00717A>
5. A meta-GGA level screened range-separated hybrid functional by employing short range Hartree-Fock with a long range semilocal functional, S. **Jana** and P. Samal, Phys. Chem. Chem. Phys., 20, 8999-9005 (2018). <http://dx.doi.org/10.1039/C8CP00333E>
6. A Parameter-Free Semilocal Exchange Energy Functional for Two-Dimensional Quantum Systems, A. Patra, S. **Jana** and P. Samal, J. Phys. Chem. A 122(13), 3455-3461 (2018). <https://pubs.acs.org/doi/10.1021/acs.jpca.8b00429>
7. Inhomogeneity induced and appropriately parameterized semilocal exchange and correlation energy functionals in two-dimensions, A. Patra, S. **Jana** and P. Samal, J. Chem. Phys. 148, 134117 (2018). <https://doi.org/10.1063/1.5019251>

Under review

8. Electronic structure calculations with the Laplacian free and asymptotic corrected semilocal exchange potential, S. **Jana**, H. Myneni and P. Samal.
9. Assessing the performance of the Tao-Mo semilocal density functional in the projector-augmented-wave method, S. **Jana**, A. Patra and P. Samal.
10. The Semilocal Exchange Hole Based meta-GGA Level Range-Separated Hybrid: Performance and Comparison with B88 Hybrids, S. **Jana**, B. Patra, H. Myneni and P. Samal.
11. Efficient lattice constants and energy band gaps for condensed systems from a meta-GGA level screened range separated hybrid functional, S. **Jana**, A. Patra, and P. Samal.
12. Performance of XDM-corrected meta-GGA level range separated hybrid on noncovalent interactions and main group thermochemistry: study within hybrids and range-separated hybrids, S. **Jana**, B. Patra, S. Swain and P. Samal.

Under preparation

13. Effect of parameters in the electronic structure calculations of bulk solids using meta-GGA level screened range separated hybrid functional, S. Jana, and P. Samal (under preparation).
14. Nonempirical meta-GGA screened hybrid functionals applied to solids, S. Jana, and P. Samal.
15. Role of kinetic energy density in the electronic structure calculations of solids.
16. Solids state assessment of Tao-Mo semilocal functional with Van-Der-Waals-Correction, A. Patra, S. Jana, and P. Samal.
17. Noneipirical meta-GGA screened hybrid functional applied to metal surfaces.

POSTER

1. S. Jana and P. Samal, "Excited-state density-functional theory revisited: study based on Hohenberg-Kohn, Gunnarsson-Lundqvist and constrained-search formalism", at Current Trends in Condensed Matter Physics 2014 (CTCMP 2015), NISER, IOP Campus, Bhubaneswar, Orissa - India (19th Feb.- 22nd Feb. 2015).
2. S. Jana and P. Samal, "Semilocal Exchange Energy Functional for Two-Dimensional Quantum Systems: A Step Beyond Generalized Gradient Approximations" (RTCMP 2017), at Recent Trends in Condensed Matter Physics 2017 (RTCMP 2017), Bose Institute, Kolkata - India (31st Oct.- 3rd Nov. 2017).
3. S. Jana and P. Samal, "Assessing the band gap problem by improving upon semilocal exchange hole" (IWAM 2017), at International Workshop on Advanced Materials 2017 (IWAM 2017), National Institute of Science and Technology (NIST), Berhampur, India and Drexel University, Philadelphia (19th Dec.- 21st Dec. 2017).

COMPUTATIONAL SKILLS

Operating systems: Linux

Programming Language: FORTRAN

Mathematical Software: Mathematica, Matlab, Origin

Electronic Structure Software: NWChem, VASP, Octopus, PWSCF (Quantum-espresso), WIEN2k, deMon2k, FHI-AIMS

TEACHING EXPERIENCE

Instructed in the Integrated M.Sc. physics laboratories. Tutored in the "Electromagnetism II", "Mathematical Physics" and "Many Body Physics" courses in NISER.

ACCOLADES

1. INSPIRE scholarship under Department of Science of Technology (DST), INDIA, (2007-2012).

REFEREES - CONTACT INFORMATION

[1] Dr. Prasanjit Samal

FC - 405 (Off.), School of Physical Sciences

National Institute of Science Education and Research (NISER), Bhubaneswar

PO- Bhimpur-Padanpur, Via- Jatni, District:- Khurda

PIN – 752050, Odisha, INDIA

Phone: +91-674-2494283, Fax: +91-674-2494262

Email: psamal@niser.ac.in , URL: <http://www.niser.ac.in/users/psamal/>

[2] Prof. Manoj Kumar Harbola

FB-476, Department of Physics

Indian Institute of Technology

Kanpur-208016, India

Phone: +91-512-259-7823

Email: mkh@iitk.ac.in, URL: <http://home.iitk.ac.in/mkh/>

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