Prasanjit Samal
(CURRICULUM VITAE)

Density-Functional Theory & Quantum Simulations Group (DFT-QSG)
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ACADEMICS:

Doctor of Philosophy **(PhD.)**, Theoretical Condensed Matter Physics,
Indian Institute of Technology (I. I. T.), Kanpur,
Kanpur-208016 (U.P.)**,** INDIA**.**

Thesis: Studies in Excited-State Density-Functional Theory

- Hohenberg-Kohn like theorem for excited-states
- Exchange-correlation functionals for excited-states
- Foundations of time-dependent density-functional theory: Floquet formulation

Professional Experience:

National Institute of Science Education and Research Bhubaneswar, INDIA
School of Physical Sciences
Assistant Professor *2009 – 2015*
Reader F *2015 - 2019*

University of Minnesota Twin Cities Campus, Minnesota
Department of Chemical Engineering and Materials Science *(CEMS) & MSI*
Postdoctoral Research Associate *2007 – 2009*

Studied the kinetics and thermodynamics of phase transformations in group-IV and II-VI nanostructures during hydrostatic or uniaxial compressions employing the ab-initio molecular dynamics simulations. The electronic-enthalpy density functional is used to carry out accurate and efficient simulations of extended as well as finite-size quantum systems under pressure.

Indian Institute of Technology Kanpur, INDIA
Department of Physics
Graduate Student Researcher *2002 – 2007*

Areas of Specialization: Density Functional Theory, Solid-State Theory, Theoretical Condensed Matter Physics, Computational Quantum Chemistry, Electronic Structure of Materials.

RESEARCH INTERESTS:

The research activity of our "DFT-QSG" 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, molecular dynamics, many-body perturbation theory and other suitable quantum many-body techniques.

The main research interest at present includes:

- Methodological developments of excited-state Density-functional theory (DFT), both static and time-dependent.
- Semi-local, non-local, global & range-separate hybrid, dielectric-dependent, exact-exchange, dispersion-corrected, exchange-correlation (XC) density-functional
- van der Waals-corrected Density Functional Theory: Surface adsorption & related Properties
- Orbital free density functional theory (OFDFT)
- Constrained Density Functional Theory (CDFT)
- Nanostructures
- Molecular & Organic Electronics
- Beyond density functional theory: GW and Bethe-Salpeter
- Material modeling
- Pseudo-potential methods in DFT
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TEACHING EXPERIENCE:

@ National Institute of Science Education and Research Bhubaneswar, INDIA

P141: Physics Laboratory I

P142: Physics Laboratory II

P201: Classical Mechanics I

P202: Mathematical Methods I

P204: Electromagnetism I

P205: Mathematical Methods II

P205: Quantum Mechanics I

P301: Electromagnetism II

P305: Atoms, Molecules and Radiation

P401: Classical Mechanics II

P451: Advanced Solid State Physics

P469: Density Functional Theory

P601: Classical Mechanics **P602: Mathematical Physics**

P603: Electromagnetism **P615: Quantum Mechanics**
@ Indian Institute of Technology Kanpur, INDIA
Graduate Student Instructor

Instructed in the **B. Tech.** and **M. Sc.** physics laboratories. Tutored in the "**Classical Mechanics**" and "**Quantum Mechanics**" courses for the period of two and one semester respectively.

PROFESSIONAL MEMBERSHIPS:

American Physical Society. Member 2007 – present

Awards and Fellowships

National Merit Scholarship, Graduate Aptitude Test of Engineering, Joint Entrance Screening Test

Skills:

Science: Very good experience of electronic-structure calculations for atomic systems. Good knowledge of wave function theory of Quantum Physics and Chemistry. Very good knowledge of "Density-Functional Theory" of ground as well as excited-states. First principle molecular dynamics.

Computer:
- Operating systems: Unix, Linux and Windows
- Programming Language: FORTRAN 77, 90, 95
- Mathematical Software: Mathematica, Matlab, Origin, Microsoft Office, Latex, Adobe Illustrator, Adobe Photoshop

Electronic Structure Software: ***ABINIT, GAMESS, GAUSSIAN, NRLMOL,*** **Octopus,** ***PWSCF (Quantum-espresso), QCHEM, SIESTA, TURBOMOLE, VASP, WIEN2k, FHI-AIMS, ADF-BAND, Molpro***

Invited Talks and Seminars:

APS March Meeting, 2008 Uniaxial compression of group-IV nanoparticles from ab-initio molecular dynamics simulations

January, 2007 Studies in Excited-State Density-Functional Theory, **I. I. T. Kanpur**

November, 2009 Hydrostatic Compression of Nanoparticles from *ab-initio*

Molecular Dynamics Simulations
Materials Workshop, Institute of Material Science, Bhubaneswar, India

Exchange Energy Functionals in Excited-State Density-Functional Theory,
Materials Workshop, Institute of Material Science, Bhubaneswar, India

March, 2011 Pressure Effect of Finite Size Nanoparticles from First Principles Molecular Dynamics, **U.G.C. "Refresher Course in Physics", Utkal University, Bhubaneswar, India**

March, 2012 Predicting Pressure Absorbing Materials through Density-Functional Theory Simulations
U.G.C. National Seminar on "Current Developments in Physics", North Orissa University, INDIA

February, 2015 Molecular dynamics simulations of nano-materials and Excited-state Functionals, **Centre for Theoretical Studies, I. I. T. Kharagpur**

August, 2015 Constrained-search formalism in excited-state DFT @ the International conference **DFT2015**, University of Debrecene, Hungary

March, 2017 Theoretical and application prospective of density-functional formalism (delivered few lectures and a seminar)
Teachers Training under QIP at Biju Patnaik University of Technology, CET, Bhubaneswar

February, 2018 meta-GGA level Semilocal Exchange-Correlation Functionals in low-dimensions, **Condensed Matter Physics Meeting, NISER**

Presented Posters:

December 2004 "Development of an exchange energy functional in excited-state density-functional theory within the local-density approximation". Theoretical Chemistry Symposium, BARC, Mumbai, India.

November 2005 Exchange energy functional in excited-state density-functional theory A National Conference to Celebrate the World Year of Physics 2005, I. I. T. Kanpur, India

December 2006 "Establishing the density-to-potential mapping in excited-state density functional theory". MESODIS 2006, I. I. T. Kanpur, India

July 2007 "Uniqueness of the density-to-potential mapping in excited-state density-functional theory".
Summer Program: Classical and Quantum Approaches in Molecular Modeling
University of Minnesota, U.S.A.

LIST of PUBLICATIONS:

1. Local-density approximation for the exchange energy functional in excited-state density-functional theory. Prasanjit Samal and Manoj K. Harbola, J. Phys. B: At. Mol. Opt. Phys. 38, 3765 (2005)

2. Density-to-potential map in time-independent excited-state density-functional theory. Prasanjit Samal, Manoj K. Harbola and A. Holas, Chemical Physics Letters, 419, 217 (2006); Erratum: Chemical Physics Letters, 422, 586 (2006)

3. Exploring foundations of time-independent density-functional theory for excited-states. Prasanjit Samal and Manoj K. Harbola, J. Phys. B: At. Mol. Opt. Phys. 39, 4065 (2006).

4. Analysis of Floquet formulation of time-dependent density-functional theory. Prasanjit Samal and Manoj K. Harbola, Chemical Physics Letters, 433, 204 (2006).

5. A local-density approximation for the exchange energy functional for excited states in bulk semiconductors: the band gap problem. M. Rahman, S. Ganguli, Prasanjit Samal, Manoj K. Harbola T. Saha Dasgupta and Abhijit Mookerjee, Physica B 404, 1137 (2009)

6. Time-independent excited-state density functional theory: study of 1s(2)2p(3)(4S) and 1s(2)2p(3) (2D) states of Boron isoelectronic series up to Ne (5+) . Manoj K. Harbola and Prasanjit Samal , J. Phys. B: At. Mol. Opt. Phys. 42, 015003 (2009).

7. Semilocal Exchange Energy Functional for Two-Dimensional Quantum Systems: A Step Beyond Generalized Gradient Approximations. Subrata Jana and Prasanjit Samal, J. Phys. Chem. A, 121, 4804(2017).

8. 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. Subrata Jana and Prasanjit Samal, J. Chem. Phys. 148, 24111(2018).

9. Inhomogeneity induced and appropriately parameterized semilocal exchange and correlation energy functionals in two-dimensions. Abhilash Patra, Subrata Jana and Prasanjit Samal, J. Chem. Phys. 148, 134117(2018).

10. Gradient approximated exchange energy functionals with improved performances for two-dimensional quantum dot systems. Subrata Jana, Abhilash Patra and Prasanjit Samal, Physica E-low-dimensional Systems & Nanostructures, 97, 268 (2018).

11. Long-range corrected density functional through the density matrix expansion based semilocal exchange hole. Bikash Patra, Subrata Jana, Abhilash Patra and Prasanjit Samal, Phys. Chem. Chem. Phys. 20, 8991 (2018).

12. A meta-GGA level screened range-separated hybrid functional by employing short range Hartree–Fock with a long range semilocal functional. Subrata Jana and Prasanjit Samal, Phys. Chem. Chem. Phys. 20, 8999 (2018).

13. A Parameter-Free Semilocal Exchange Energy Functional for Two-Dimensional Quantum Systems. Abhilash Patra, Subrata Jana and Prasanjit Samal, J. Phys. Chem. A. 122, 3455 (2018).

14. Assessing the performance of the Tao-Mo semilocal density functional in the projector-augmented-wave method, S. Jana, A. Patra and P. Samal, J. Chem. Phys. 149, 044120 (2018). https://doi.org/10.1063/1.5040786

15. 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, J. Chem. Phys. 149, 094105 (2018). https://doi.org/10.1063/1.5037030

16. Assessing the performance of the recent meta-GGA density functionals for describing the lattice constants, bulk moduli, and cohesive energies of alkali, alkaline-earth, and transition metals, S. Jana, K. Sharma, and P. Samal, J. Chem. Phys. 149, 164703 (2018). https://doi.org/10.1063/1.5047863

17. On the many-electron self-interaction error of the semilocal exchange hole based meta-GGA level range-separated hybrid with the B88 hybrids, S. Jana, B. Patra, H. Myneni, and P. Samal, Chem. Phys. Lett. Volume 713, Pages 1-9 (2018). https://doi.org/10.1016/j.cplett.2018.10.007

18. Screened hybrid meta-GGA exchange-correlation functionals for extended systems, S. Jana and P. Samal, Phys. Chem. Chem. Phys., 21, 3002-3015 (2019). http://dx.doi.org/10.1039/C8CP06715E

19. Long-range screened hybrid functional theory satisfying the local density linear response, S. Jana, A. Patra, L. A. Constantin, H. Myneni and P. Samal, Phys. Rev. A, (2019).

20. Colle-Salvetti type correlation functionals for two-dimensional quantum dot systems, A Patra, P Samal Chemical Physics Letters 720, 70-75 (2019)

21. Improving the performance of Tao-Mo non-empirical density functional with broader applicability
in quantum chemistry and material sciences, S. Jana, K. Sharma, and P. Samal. (J. Chem. Phys.)
https://arxiv.org/abs/1808.09937

22. Parametric Influence On The Electronic Structure Calculations Of Solids Using meta-GGA Level
Screened Range-Separated Hybrid Functional, S. Jana, and P. Samal.

Ongoing Research Projects

23. Density-functional study of spin-flip/charge-transfer excitations in finite and extended systems. Prasanjit Samal

24.Studying Pauli and Coulomb Correlations in Excited-State Density-Functional Theory. Prasanjit Samal

25. Constrained search formalism in TDDFT, Subrata Jana, Bikash Patra and Prasanjit Samal

26. Laplacian free and asymptotic corrected semilocal exchange potential applied to band gap of solids, A. Patra, S. Jana, H. Myneni, and P. Samal.

27. Modified exchange hole with the application of the efficient band gap prediction for solids, B. Patra, S. Jana, and P. Samal.

28. PBEint exchange-correlation and local density linear response based screened range-separated hybrid for solid-state materials, S. Jana, A. Patra, L. A. Constantin and P. Samal.

29. Generating the pseudopotential and assessing the performance of the accurate meta-GGA functional in the plane-wave pseudopotential code Quanum Espresso, B. Patra, R. Singh, S. Jana, and P. Samal.

30. Role of Kohn-Sham kinetic energy density in the electronic structure calculations of solids, S. Jana, K.Sharma, and P. Samal.

31. Performance of semilocal density functional for the surfce, work function and adsorption in metallic surfaces, S. Jana, A. Patra, K. Sharma and P. Samal.

32. Performance of the modified semilocal functional in quantum chemistry, S. Jana, B. Patra, S. Jana, and P. Samal.

33. Non-empirical meta-GGA screened hybrid functional applied to the bulk and surface properties of metals and metallic surfaces, S. Jana, K. Sharma and P. Samal.

34. First principle phonon calculation from meta-GGA level semilocal and screened hybrid functional theory. S. Jana, and P. Samal.

35. Semiclassical atom theory and local density linear response based screened range-separated hybrid functional applied to the solid-state materials, A. Patra, S. Jana, L. A. Constantin, and P. Samal.

36. Long-range corrected PBE functional by satisfying local density linear response, S. Jana, L. A. Constantin, and P. Samal.

37. Quasi-2D GGA functional for the surface energy and work function of solids, S. Jana, L. A. Constantin, and P. Samal.

38. Assymptotic corrected SCAN meta-GGA functional, S. Jana, and P. Samal.

39. Excitation energy from a modified semilocal functional, S. Jana, and P. Samal.

40. Meta-GGA range seperated hybrid functional theory applied to the excitation energy of molecules, B. Patra, S. Jana, and P. Samal.

41. Modified Becke-Roussel exchange hole potential to propose long-range corrected, screened hybrid functional for the molecular systems and solid state system, B. Patra, S. Jana, and P. Samal.

42. Uniaxial compression of group-IV nanoparticles from ab-initio molecular dynamics simulations. Prasanjit Samal *and* Matteo Cococcioni, (in preparation).

43. Time-independent excited-state DFT through Legendre transformation Prasanjit Samal (in preparation)

44. Excited-state density-functional theory revisited: study based on Hohenberg-Kohn, Gunnarsson-Lundqvist and constrained-search formalism, Prasanjit Samal, Subrata Jana & Sourabh S. Chauhan (Unpublished).

Review articles & Book Chapters

Time-independent excited-state density functional theory AIP Conference Proceedings 1108, 54 (2009).
Excited-state density functional theory, XXVII International Conference on Photonic, Electronic and Atomic Collisions, Belfast, (2011)
Excited-state density functional theory J. Phys.: Conf. Ser. (2012)
Energy functionals for excited states, Concepts and Methods in Modern Theoretical Chemistry, Vol. 1: Electronic Structure and Reactivity (2014)

Conference Organized

Current Trends in Condensed Matter Physics (CTCMP), 2010, 2015
http://www.niser.ac.in/~ctcmp2010/