

Rabeet Singh

November 10, 2019

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Date of Birth - 5th July 1990

Nationality - Indian

Civil State - Single

ORCID iD

ResearchGate

Google Scholar

Experience

From Dec 27, 2017 to Present

Post - Postdoctoral Fellow

Institute - National Institute of Science Education and Research

Main Activity - Research

Mentor - Dr. Prasanjit Samal

Achieved Degrees

From July 2012 to May 2018

Degree - Ph.D. (Physics), CGPA : 8.64 out of 10

Institute - Indian Institute of Technology Kanpur, Kanpur

Serial No. : PG-61N535RK

Thesis Title - Adiabatic connection in density functional theory: Fundamental aspects and applications

Thesis Supervisor - Prof. Manoj Kumar Harbola

From July 2010 to April 2012

M.Sc. (Physics) , CGPA : 6.51 out of 10

Indian Institute of Technology Delhi, Delhi

Entry No. - 2010PHS7027

From July 2007 to July 2010

B.Sc. (Physics, Chemistry, Mathematics), Percentage : 67.9%

M.J.P Rohilkhand University, Bareilly

Enrol. No. - 0757723

Research

I am interested in exploring and developing wavefunction and density-based methods for solving many-electron systems.

Manuscripts

Published

- Rabeet Singh and Manoj K. Harbola, "Improved Le Sech wavefunctions for two-electron atomic systems". Chem. Phys. Lett. **639**, 248(2015).
- Rabeet Singh and Manoj K. Harbola, "Study of adiabatic connections in density functional theory for 2-electron spherical systems". Int. J. Quantum Chem. **117**, 25344(2017)
- Rabeet Singh and Manoj K. Harbola, "A study of accurate exchange-correlation functionals through adiabatic connection". J. Chem. Phys. **147**, 144105(2017)
- Ashish Kumar, Rabeet Singh, and Manoj K. Harbola, "Universal nature of different methods of obtaining the exact Kohn-Sham exchange-correlation potential for a given density". J. Phys. B **52**, 075007(2019)

Accepted

- Rabeet Singh, Ashish Kumar, Manoj K. Harbola, and Prasanjit Samal, "Accurate wavefunctions and Kohn-Sham exchange-correlation potentials for two-electron atomic systems in two-dimensions." (*Provisionally accepted, J. Phys. B*)
- Rabeet Singh, Bikash Patra, Abhilash Patra, Manoj K. Harbola, and Prasanjit Samal, "Adiabatic connection in density functional theory in two-dimensions: A semi-analytic wavefunction based study for two-electron atomic systems" (*Accepted, J. Chem. Phys.*)

Submitted

- Ashish Kumar, Rabeet Singh, and Manoj K. Harbola "Accurate effective potential for density amplitude and the corresponding Kohn-Sham exchange-correlation potential calculated from approximate wavefunctions" (*Under review, J. Chem. Phys*)

Under Preparation

- Rabeet Singh and Manoj K. Harbola, "The Levy-Perdew-Sahni equation for the density: accurate effective potential and self-consistent solution for two-electron atomic systems". (<https://arxiv.org/pdf/1602.07042.pdf>)
- Rabeet Singh, Subrata Jana, and Prasanjit Samal, "Performance of recently developed meta-GGA exchange-correlation functionals in density functional theory for calculating lattice dynamical properties of group-IV semiconductors"
- Rabeet Singh, Bikash Patra, Subrata Jana, and Prasanjit Samal, "The localized dynamical correlation applied to accurate semilocal density functional."
- Rabeet Singh, Ashish Kumar, and Manoj K. Harbola, "Studying the exchange-correlation hole during the adiabatic connection in density functional theory for two-electron atomic systems."
- Bikash Patra, Rabeet Singh, Subrata Jana, and Prasanjit Samal "Construction of Norm-conserving pseudopotentials for the accurate semilocal functionals"

Computer Skills

■ Programming Languages

Fortran, C, Python, html, Parallel-programming in openmp

■ Calculation Tools

VASP (For bulk systems), NWChem (For atoms and molecules), QUANTUM ESPRESSO (For bulk systems), DFTATOM (For getting basic subroutines), LIBXC (For using exchange-correlation functionals), APE and ld1.f90 (For generating Pseudopotentials) Mathematica (For deriving and checking analytical expressions) cif2cell, and atomsk (For generating input files to perform electronic structure calculations)

■ Writing tools

Latex (mostly in textstudio), Vim

■ Plotting Tools

Gnuplot, Pgfplot, and Latexdraw

■ Visualization Tools

Xcrysden p4vasp, and Vesta

■ Miscellaneous

Linux, Shell Script-writing, Makefile.

Conferences & Schools attended

- EMN Meeting on Computation and Theory 2017, Dubai, UAE.
- Hands on Training on Multiscale Simulation in Advanced Materials Science & Technology (HTMSAMST-2016) July 14-24, 2016, Department of Applied Physics, S. V. National Institute of Technology, Surat, INDIA
- Current Trends in Condensed Matter Physics (CTCMP 2015) held at National Institute of Science Education and Research, Bhubaneswar (February 19-22, 2015).
- Summer School on Materials Simulation Theory and Numerics (MASTANI) at IISER, PUNE on July 2014.
- ICTS School and Discussion Meeting on Strongly Correlated Systems: From Models to Materials at the Deptt. Of Physics, IISc. , Bangalore (January, 2014).
- Recent Trends in Nanophotonics, October, 2011 at IIT Delhi.

Prize

- Prof. V. K. Saxena memorial science test, Second Prize (2010) at Bareilly College, Bareilly.

Teaching Experiences

- Worked as a Teaching Assistant in PHY101(B.Tech Lab), PHY102(Introductory Mechanics) and PHY103 (Introduction to Electromagnetism) courses at IIT Kanpur.
- Worked as a Teaching Assistant for the following on-line courses run through the National Program on Technology Enhanced Learning (NPTEL) by Prof. Manoj K. Harbola,
 1. Introduction to Electromagnetism (Jan-April, 2015)
 2. Introduction to Electromagnetic Theory (July-Sep, 2016)
 3. Engineering Mechanics (July-Oct, 2016)
 4. Introduction to Quantum Mechanics (Jan-March, 2017).

Hobbies

- **Cycling, Swimming, Traveling, Cricket, Script Writing**

Referees

Name - Prof. Manoj K. Harbola
Institute - Indian Institute of Technology Kanpur
Position - Professor
Email - mkh@iitk.ac.in

Name - Prof. Amit Agarwal
Institute - Indian Institute of Technology Kanpur
Position - Assistant Professor
Email - amitag@iitk.ac.in

Name - Dr. Prasanjit Samal
Institute - National Institute of Science
Education and Research
Position - Reader
Email - psamal@niser.ac.in

Name - Prof. Rajeev Gupta
Institute - Indian Institute of Technology Kanpur
Position - Professor
Email - guptaraj@iitk.ac.in