Ankit Mahajan

Contact Information

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Research Interests

I am interested in electronic structure techniques in **quantum chemistry** and **condensed matter physics**. Recently, I have been working on developing Quantum Monte Carlo methods to study strongly correlated systems.

Education

Indian Institute of Technology, Bombay (IITB), Mumbai, India

5 Year Integrated MSc in Physics — July 2012 - April 2017
Minor in Computer Science and Engineering

University of Colorado, Boulder, CO USA

PhD student in Chemical Physics — August 2017 -
Advisor: Sandeep Sharma, Department of Chemistry, University of Colorado, Boulder

Publications

Mahajan, A. and Sharma, S., Symmetry-projected Jastrow mean-field wave function in variational Monte Carlo. *The Journal of Physical Chemistry A,* **123(17)** 2019, arXiv:1902.07690.

Mahajan, A., Blunt, N.S., Sabzevari, I. and Sharma, S., Multireference configuration interaction and perturbation theory without reduced density matrices. *The Journal of Chemical Physics,* **151(21)** 2019, arXiv:1909.06935 (**Featured article**).

Sabzevari, I., **Mahajan, A.** and Sharma, S., An accelerated linear method for optimizing nonlinear wavefunctions in variational Monte Carlo. *The Journal of Chemical Physics,* **152(2)** 2020, arXiv:1908.04423.

Blunt, N.S., **Mahajan, A.** and Sharma, S., Efficient multireference perturbation theory without high-order reduced density matrices. *The Journal of Chemical Physics,* **153(16)** 2020, arXiv:2008.00220.

Mahajan, A. and Sharma, S., Efficient local energy evaluation for multi-Slater wave functions in orbital space quantum Monte Carlo. *The Journal of Chemical Physics,* **accepted** 2020, arXiv:2008.06477.

Talks

Nonlinear Dynamics of Hodgkin-Huxley Neurons — November, 2014
Supervised learning presentation, Department of Physics, IIT Bombay

Extrapolation techniques to improve the scaling of electronic structure — April, 2017
Condensed matter theory presentation, Department of Physics, IIT Bombay

Correlations and symmetry in mean-field wave functions — February, 2019
Theory supergroup meeting, Department of Chemistry, CU Boulder

Jastrow multi-Slater electronic wave functions — September, 2020
Theory supergroup meeting, Department of Chemistry, CU Boulder

Teaching

Teaching assistant or grader

- **University of Colorado, Boulder:** Physical Chemistry (CHEM 4511 and 4531), General Chemistry (CHEM 1113 and 1133).
- **Indian Institute of Technology, Bombay:** Calculus (MA 105), Electricity and Magnetism (PH 103).

Scholastic Achievements

- National Talent Search Examination (NTSE) 2009 scholarship by Govt. of India.
- Kishore Vaigyanik Protsahan Yojana (KVPY) 2012 fellowship by Department of Science and Technology, Govt. of India.
- Secured All India Rank 931 in IIT Joint Entrance Examination (JEE) 2012 among about 500,000 candidates.
- Secured All India Rank 406 in All India Entrance Examination (AIEEE) 2012 among over a million candidates.
- KPMG Scholarship 2014, based on excellent academic performance in freshman year.
- Sharrah Graduate Fellowship 2019, Department of Chemistry, University of Colorado, Boulder.

Technical skills

- Programming languages: C/C++, Python, Mathematica, Java
- Web: HTML, CSS, JS, JSP
- Software packages: Autocad, Arduino IDE, MySQL