

Ankit Mahajan

CONTACT INFORMATION

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RESEARCH INTERESTS

I am interested in **condensed matter physics** and **quantum chemistry**, specifically in computational electronic structure theory. My other interests include nonlinear dynamics and quantum computing.

EDUCATION

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

5 Year Integrated MSc in Physics *July 2012 - April 2017 (Expected)*
(converted from BTech Engineering Physics in *July, 2015*)
Minor in Computer Science and Engineering
Cumulative Performance Index: **8.9** on 10

TEST SCORES

General GRE: **334/340** (Verbal: 164/170, Quantitative: 170/170, Writing: 4.0/6.0)
Physics GRE: **990/990**
TOEFL: **111/120** (Reading: 30/30, Listening: 28/30, Speaking: 26/30, Writing: 27/30)

RESEARCH EXPERIENCE[†]

Master's Thesis: *Ab initio* molecular dynamics using fragment-based electronic structure theory *July, 2016 - Ongoing*

Guide: Prof. Srinivasan Iyengar, Indiana University, Bloomington

Co-guide: Prof. Aftab Alam, IIT Bombay

I am studying the applications of a fragment-based electronic structure method, PIE-ONIOM, to *ab initio* molecular dynamics. I have learned about two composite quantum chemical approaches, *viz.* hybrid methods (QM/MM, ONIOM) and fragment-based methods (FMO, MTA), through a literature survey. I have modified the existing PIE-ONIOM wrapper code to allow combinations of different electronic structure packages. Our goal is to study the applicability of DMRG within the PIE-ONIOM approach for both static and dynamics calculations.

BTech Project: DMRG calculations of π -conjugated oligomers within the Pariser-Parr-Pople model *July, 2015 - July, 2016*

Guide: Prof. Alok Shukla, IIT Bombay

In the first phase, I studied the basics of electronic structure theory including plane wave methods, tight binding, HF, CI, etc. in the second quantized formalism. In the second phase, I learned the theory of Density Matrix Renormalization Group using Matrix Product States. We did benchmark DMRG-CI calculations of π -conjugated oligomers (t-PA, polyacenes, PPP, trigonal quantum dots) starting with the HF orbitals of the Pariser-Parr-Pople Hamiltonian. The DMRG-CI energies were found to compare favorably FCI, QCI and MRSDCI results, wherever applicable. A publication based on these results is under preparation.

Summer Internship: Quantum Wavepacket *Ab Initio* Molecular Dynamics (QWAIMD) on an adaptive, moving grid *Summer 2015*

Guide: Prof. Srinivasan Iyengar, Indiana University, Bloomington

I studied various techniques of *on-the-fly ab initio* molecular dynamics, with focus on Atom Centered Density Matrix Propagation. I learned about the hydrodynamical formulation of quantum dynamics (Bohmian mechanics). QWAIMD treats one nucleus in the system quantum mechanically by propagating a wave-packet on a grid. We worked out the theory of a grid moving with the

wave-packet using Pullay forces. I was able to modify the QWAIMD FORTRAN code to implement an adaptive, vibrating grid using Distributed Approximating Functionals (DAF).

Supervised Learning Project: Simulating the response of a Hodgkin-Huxley neuron cable to an external electromagnetic field *July, 2014 - November, 2014*

Guide: Prof. Punit Parmananda, IIT Bombay

I learned about the Fitzhugh-Nagumo and Hodgkin-Huxley models of neuronal activity. We modified the HH cable equations, a set of four coupled, nonlinear partial differential equations, to include the effects of a time dependent EM field. The system was numerically integrated using MATLAB. We found that certain frequencies of the EM field can elicit an action potential response. Presence of an Arnold tongue in the forcing amplitude-frequency parameter space was demonstrated.

PAPER IN
PREPARATION[†]

A paper titled **DMRG calculations of π -conjugated oligomers within the Pariser-Parr-Pople model** is under preparation in collaboration with Prof. Alok Shukla.

KEY COURSE
PROJECTS[†]

Gauge kinematics of deformable bodies *Spring 2015*

Guide: Prof. Ravi Banavar, IIT Bombay

Course: Differential geometric methods in control

I reviewed the paper, similarly titled, authored by Wilczek and Shapere. I studied the concepts of connections and parallel transport on principal fiber bundles. These structures, which provide a natural setting for describing dynamics of everyday deformable objects (a falling cat, for example), are ubiquitous in the gauge theories fundamental physical interactions. This problem provides a clearer view of the concepts involved compared to the abstract formulations of fundamental physical laws.

Superconductivity as a broken $U(1)_{EM}$ symmetry *Spring, 2015*

Guide: Prof. Urjit Yajnik, IIT Bombay

Course: Special topics in particle physics (Advanced QFT)

I learned how gauge symmetries arise in the formulation of fundamental interactions and lend them a geometric meaning. I examined the Goldstone theorem and the way Higgs mechanism solves the problem of gauge field masses. I also studied how the spontaneous breaking of electromagnetic $U(1)$ gauge symmetry of the Ginzburg-Landau Hamiltonian can be used to explain the exotic properties exhibited by superconductors, like Meissner effect, flux quantization, etc.

Frequency analysis of audio signals (in a group of 3) *Autumn 2014*

Guide: Prof. Pradeep Sarin, IIT Bombay

Course: Microprocessor and digital electronics lab

We designed a real-time audio frequency analyzer using the ATMEGA microcontroller. Mic output was amplified using an opamp circuit and connected to the MCU. A fast Fourier transform of the discretized signal would be carried out and displayed on a screen in real time (functional for frequencies up to 28 kHz).

Movie database web application (in a group of 2) *Autumn 2014*

Guide: Prof. Umesh Bellur, IIT Bombay

Course: Database and information systems

We designed a web-enabled movie database based on the MVC architecture. The *model* part consisted of a Java application connected to a MySQL database through the JDBC API. JSP's were used for the *view*, to create dynamic web pages, and Java servlets worked as *controllers*. Functionalities implemented included listing all the movies starring an actor, awards won by a movie, etc.

[†] Reports and additional details can be found on my [homepage](#).

TEACHING
EXPERIENCE

Teaching assistant for MA 105 Calculus

Autumn 2016

Tutor for a batch of 48 first year undergraduate students. My duties as a TA included conducting weekly hour-long tutorials for resolving theory doubts, solving problems and grading examination papers.

SCHOLASTIC
ACHIEVEMENTS

- **Department rank 4** out of 43 Engineering Physics students before converting to integrated MSc.
- One of only two students to receive the top grade in the graduate level course *Nonlinear Dynamics*, one of three in *Quantum Computing*, *Lie Groups and Lie Algebras* and *Differential Geometric Methods in Control*.
- Awarded the KPMG scholarship 2013, to cover tuition expenses for a year, based on excellent academic performance in freshman year.
- Secured **All India Rank 931** in IIT Joint Entrance Examination (JEE) 2012 among about 500,000 candidates.
- Secured **State Rank 33** and **All India Rank 406** in All India Entrance Examination (AIEEE) 2012 among over 1 million candidates.
- Qualified for Kishore Vaigyanik Protsahan Yojana (KVPY) 2012 fellowship by Department of Science and Technology, Govt. of India.
- One among top 1000 students nationwide to be awarded the National Talent Search Examination (NTSE) 2012 scholarship by Govt. of India.

TECHNICAL SKILLS

- Programming languages: Extensive use of C/C++, Fortran, BASH, TCSH, MATLAB. Some experience with Java, Python, Mathematica, MySQL.
- Quantum Chemistry Packages: Gaussian, Psi4, Orca, Gamess UK, Tinker, Molden, VMD
- Web: HTML, CSS, JS, JSP
- Software packages: L^AT_EX 2_ε, Autocad, MS Office, Arduino IDE
- Operating Systems: Unix/Linux, Windows

REFERENCES

- **Prof. Srinivasan Iyengar** (Senior thesis and summer internship guide)
Department of Chemistry, Indiana University, 800 E Kirkwood Ave, Bloomington, IN 47405, United States
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- **Prof. Alok Shukla** (BTech project guide and course instructor)
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- **Prof. Aftab Alam** (Project guide and course instructor)
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