Srimukh Prasad Veccham

Research Interests: Development of theoretical models and computational techniques and applying them to chemical systems

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Education

2015 – 2020 (expected)	**University of California Berkeley,** Berkeley, CA Candidate for Ph.D in Physical Chemistry | GPA: 3.95/4 Advisor: Prof. Martin Head-Gordon
2010 – 2015	**Indian Institute of Technology Bombay,** Mumbai, India Masters of Science in Chemistry | GPA: 9.29/10 Minor in Electrical Engineering Ranked #1 in Department of Chemistry

Current Research Projects

UniRep++
Deep learning models implemented in TensorFlow. Regex and pandas used for data manipulations and analysis. Code available on Github

- Built a model to identify the role of active site residues in protein function from protein sequence information with 88% accuracy
- Used a multi-scale representation for the whole system consisting of a modified RNN based representation for the protein sequence and message passing neural network based representation for the active site residue
- Achieved 90% accuracy in identifying the function of enzymes by predicting the enzyme commission number

Polarized Many-Body Expansion
Central computation engine implemented in C++ with end-to-end Python wrappers for creation, execution, and collection of computation processes on high performance computing architectures

- Formulated a computationally inexpensive technique to compute molecular energies and properties using Density Functional Theory (DFT)
- Formal complexity reduced from $\mathcal{O}(N^3)$ to $\mathcal{O}(N^2)$, providing speedups of 10 to 100 times
- Algorithm is "embarrassingly parallelizable," practically achieving perfect scaling upto 64 processors
- Demonstrated the success of this technique in over 50 molecular systems with errors
- Currently working on extensions to correlated wavefunction methods

Performance of Density Functionals for Hydrogen Storage
Implemented Python wrappers for spawning jobs using Q-Chem, MRCC, and Psi4. Used Pandas for data analysis and interpretation

- Compiled a dataset of 275 data points to accurately represent the hydrogen storage problem in porous materials
- Assessed the performance of over 55 density functionals against the reference binding energies
- Identified density functionals which can predict hydrogen binding energies with about 3% error
- Reduced computational cost by upto 1000 times in predicting binding energies
- Generated and curated over 30,000 data points with different meta data structures over the course of this project

Variational Decomposition of Pair-wise Charge Transfer
Implemented numerical quadrature algorithms and iterative algorithms for non-linear objective function optimization in C++ using Armadillo

- Implemented a variational alternative to the perturbative pair-wise charge decomposition in Energy Decomposition Analysis scheme
- Analyzed and carefully characterized the physical interpretation of each of the charge transfer terms such that charge transfer is comprehensively categorized

Publications

- **Srimukh Prasad Veccham,** Joonho Lee, Martin Head-Gordon "Making Many-Body Interactions Nearly Pairwise Additive: The Polarized Many-Body Expansion Approach" *J. Chem. Phys.* 2019, 151, 194101
- **Srimukh Prasad Veccham,** Martin Head-Gordon "Density Functionals for Hydrogen Storage: Defining the H2Bind275 Test Set with Ab Initio Benchmarks and Assessment of 55 Functionals" *Submitted to Journal of Chemical Theory and Computation*
- **Srimukh Prasad Veccham,** Joonho Lee, Martin Head-Gordon "Variational Charge-Transfer Analysis in ALMO-based Energy Decomposition Analysis" *Manuscript in preparation*
- Mark D. Allendorf, Zeric Hulvey, Thomas Gennett, ... **Srimukh Prasad Veccham,** Brandon C. Wood "An assessment of strategies for the development of solid-state adsorbents for vehicular hydrogen storage" *Energy & Environmental Science* 2018, 11, 2784
- E. Tsivion, **Srimukh Prasad Veccham,** Martin Head-Gordon "High-Temperature Hydrogen Storage of Multiple Molecules: Theoretical Insights from Metalated Catechols" *Chem. Phys. Chem.* 2017, 18, 184
- Sajesh P. Thomas, **Srimukh Prasad Veccham,** Louis J. Farrugia, Tayur N. Guru Row "'Conformational Simulation' of Sulfamethizole by Molecular Complexation and Insights from Charge Density Analysis: Role of Intramolecular S···O Chalcogen Bonding" *Crystal Growth* & Design 2015, 15, 2110

Conference Presentations

Variational Pairwise Charge Transfer Decomposition in ALMO-based Energy Decomposition Analysis August, 2021
Accepted for poster presentation at the 12th Triennial Congress of the World Association of Theoretical and Computational Chemists

Polarized Many-body Expansion: A Perfect Marriage between Embedded Mean-field Theory and Variational Many-body Expansion April, 2019
Oral presentation at the Spring National Meeting of the American Chemical Society, Orlando, FL

Assessment of the Performance of Density Functionals for Hydrogen Storage in Sorbents April, 2019
Oral presentation at the Spring National Meeting of the American Chemical Society, Orlando, FL

Polarized Many-Body Expansion May, 2019
Poster presentation at the Northern California Theoretical Chemistry Meeting, Berkeley, CA

Awards and Honors

Institute Silver Medal for highest GPA in Department of Chemistry, IIT Bombay — August, 2015
Young researcher at 65th Lindau Nobel Laureate Meeting, Lindau, Germany — June, 2015
Institute Academic Prize for highest GPA in each semester for 6 semesters — July, 2011 – May, 2014
Summer Undergraduate Research Fellowship awarded Duke University — May, 2013
Summer Research Fellowship awarded by Indian Academy of Sciences — May, 2012
INSPIRE fellowship by Department of Science & Technology, Government of India — July, 2010 – May, 2015

Skills

Scientific programming:	Extensive production-level programming experience in Q-Chem, a comprehensive electronic structure package. Contributed to embedding and energy decomposition analysis libraries.
Software and packages:	TensorFlow, PyTorch, Gaussian, Psi4, RDKit, NAMD, GROMACS, VMD, NBO, ChemOffice, MRCC LaTeX
Programming languages:	C++ (Armadillo), Python (NumPy, SciPy, Pandas, Matplotlib)

Relevant Coursework

- **Computer science**: Machine Learning, Machine Learning in Chemistry and Biology , Computer Programming and Utilization
- **Mathematics/Statistics**: Vector Calculus , Linear Algebra , Differential Equations , Data Analysis and Interpretation , Probability and Random Processes
- **Numerical methods**: Advanced Simulation Techniques in Physics , Numerical Solutions to Differential Equations (audit) , Advanced Matrix Computations (audit)

- **Chemistry**: Advanced Quantum Mechanics I , Advanced Quantum Mechanics II , Thermodynamics and Statistical Mechanics , Chemical Kinetics

Teaching Experience

Upper Division Physical Chemistry Spring 2017, UC Berkeley

- Lead discussion sections and formulated and graded assignments and exams

Freshman General Chemistry Fall 2015, 2016 UC Berkeley

- Lead a laboratory section, solved tutorial problems and lead discussion sections
- Graded laboratory reports, assignments, quizzes, and exams with feedback

Freshman Physical Chemistry Spring 2014, IIT Bombay

- Lead discussion section, solved tutorial problems, and handled student questions