Srimukh Prasad Veccham

Research Interests: Development and application of machine learning models to understand physical systems

42 Gilman, University of California
Berkeley, CA 94270
srimukh.prasad@berkeley.edu
(510)944-2140
srimukhp.github.io

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. Manuscript available on request.

- Built a model to identify the role of active site residues in an amino acid 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
- Created a novel representation for amino acid residues called "embedded" one-hot encoding representation for amino acid residues, a simple and powerful technique to encode environment information into amino acids
- 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

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
- Conceptualized a scheme that is chemically grounded with correct discretization limits
- This scheme can decompose 100% of the interaction energies as opposed to $\sim$70%

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" *J. Chem. Theory Comput. In press*
- **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

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, Psi4, MRCC, Gaussian, NAMD, GROMACS, VMD, NBO, ChemOffice, 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