Osman **Mamun**

Chemical Engineer · Computational Catalysis · Machine Learning

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Education

University of South Carolina — *Columbia, South Carolina*

PhD in Chemical Engineering — *Aug. 2012-Aug. 2017*

CGPA: 3.79/4.00

Bangladesh University of Engineering & Technology (BUET) — *Dhaka, Bangladesh*

B.S. in Chemical Engineering — *Jun. 2007-Feb. 2012*

CGPA: 3.79/4.00

Professional Experience

Stanford University — *Menlo park, California*

Postdoctoral scholar — *Sep. 2017-present*

Advisor: Dr. Thomas Bligaard

- Developed a machine learning model to predict the adsorption energies of multi-atom monodentate hydrogenated species on bimetallic alloy surfaces with a MAE of 0.1 eV for mono-hydrogen species and 0.2 eV for multi-hydrogen species
- Developed a graph theoretic approach to high-throughput enumeration of surface structure generation for up to C3 species and transition structure generation for up to C2 species (ongoing work to make it more robust and extensible)
- Developing an active learning framework to reduce the number of expensive NEB computation that identifies and submits potentially important computation based on Gaussian Process inference.
- Developed a database of surface chemical reactions that is made freely available for the catalysis community for data validation, model generation etc.
- Developed a machine learning classifier to identify potentially unstable adsorbate-surface complex to reduce the waste of massive computational resources.By maximizing the precision (at the expense of recall), I ensured that no stable structures are omitted.

University of South Carolina — *Columbia, South Carolina*

Graduate Research Assistant — *Aug. 2012-Aug. 2017*

Advisor: Prof Andreas Heyden

- Investigated the vapor and liquid phase kinetics of Levulinic acid on Ru surface catalysts. Based on my research, I identified polar solvent, e.g., water, and high temperature are the predominant factors affecting the reaction kinetics.
- Performed first-principles kinetic Monte Carlo simulation and microkinetic analysis of the hydrogenation of various ketones and aldehydes over Ru(0001) to accurately consider lateral interaction effect on the reaction kinetics. My study found that lateral interaction effect is negligible to describe the reaction kinetics for ketone hydrogenation on Ru(0001) surfaces.
- Performed theoretical investigation (QM/ML approach using Gaussian Process Regression) of the distribution of carbohydrates in various liquid phase environments. Based on the theoretical isomer distribution, experimentalists at Syracuse University developed reaction kinetics model for sugar conversion reactions.
- Worked as TA for several graduate and undergraduate level courses.

Publications

Google scholar profile: https://scholar.google.com/citations?user=NJdTPhkAAAAJ&hl=en

1. **Mamun O.**, Walker E., Faheem M., Heyden A. "Theoretical Investigation of the Hydrodeoxygenation of Levulinic Acid to γ-Valerolactone over Ru(0001)" ACS Catalysis 7 (1), 215-228
2. **Mamun O.**, Saleheen S., Bond J. Q., Heyden A. "Importance of Angelical Lactone Formation in the Hydrodeoxygenation of Levulinic Acid to γ-Valerolactone over Ru catalysts" Journal of Physical Chemistry C 121(34), 18746-18761
3. Lu J., Behtash S., **Mamun O.**, Heyden A. "Theoretical Investigation of the Reaction Mechanism of the Guaiacol Hydrogenation over a Pt (111)" ACS Catalysis 5 (4), 2423-2435
4. Behtash S., Lu J., Walker E., **Mamun O.**, Heyden A. "Solvent effects in the liquid phase hydrodeoxygenation of methyl propionate over a Pd (111) catalyst model" Journal of Catalysis 333, 171-183
5. Behtash S., Lu J., **Mamun O.**, Williams CT., Monnier JR., Heyden A. "Solvation Effects in the Hydrodeoxygenation of Propanoic Acid over a Model Pd(211) Catalyst" Journal of Physical Chemistry C 120(5),2724-2736
6. Chowdhury A., Yang W., Walker E., **Mamun O.**, Heyden A., and Terejanu G. "Prediction of Adsorption Energies for Chemical Species on Metal Catalyst Surface Using Machine Learning" Journal of Physical Chemistry C 122(49), 28142-28150 **ACS Editor's Choice Article**
7. Boes J. R., **Mamun O.**, Winther K., Bligaard T. "Graph Theory Approach to High-Throughput Surface Adsorption Structure Generation" Journal of Physical Chemistry A 123(11), 2281–2285
8. **Mamun O.**, Chowdhury A., Gabriel T., Bond J. Q., Heyden A. "Towards Quantum Mechanical Predictions of Carbohydrate Isomer Distribution via Machine Learning" – In preparation
9. **Mamun O.**, Saleheen S., Bond J. Q., Heyden A. "Investigation of Solvent Effects on the Hydrodeoxygenation of Levulinic Acid over Ru(0001)" – submitted
10. Winther K., Hoffmann M. J., Boes J. R., **Mamun O.**, Bajdich M., Bligaard T. "Catalysis-Hub.org: An Open Electronic Structure Database for Surface Reactions" Scientific Data 6 (75), 2019
11. **Mamun O.**, Winther K., Boes J., Bligaard T. "High-throughput Calculations if Catalytic Properties of Bimetallic Alloy Surfaces" Scientific Data 6(75), 2019
12. **Mamun O.**, Boes J. R., Winther K., Hansen M. H., Bligaard T. "A Delta Learning Approach to High-Throughput Adsorption Energy Prediction on Bimetallic Alloy Catalysts" – Submitted
13. Hansen M., Torres J., Jennings P., Wang Z., Boes J., **Mamun O.**, Bligaard T. "CatLearn - an Atomistic Machine Learning Package for Surface Science and Catalysis" – Submitted

Dissertation

- Theoretical Investigation of the Catalytic Hydrodeoxygenation of Levulinic Acid over Ru(0001) Catalytic Surface. (Link: https://scholarcommons.sc.edu/etd/4269)

Conference presentation

1. "Rational design of bifunctional catalysts for the conversion of levulinic acid to γ-valerolactone" **Mamun O.**, Faheem M., Heyden A., AIChE Annual Meeting, Atlanta, GA, November 2014.
2. "Theoretical Investigation of the Vapor Phase Kinetics of the Hydrodeoxygenation of Levulinic Acid over Ru (0001): A combined DFT and Microkinetic Modelling Study" **Mamun O.**, Heyden A., Annual Chemical Engineering Symposium, Chemical Engineering Dept., University of South Carolina 2014
3. "Theoretical Investigation of the Hydrogenation of Levulinic Acid over Ru Catalysts" **Mamun O.**, Omar A., Bond J. Q., Heyden A. AIChE Annual Meeting, Salt Lake City, Utah, November 2015.

4. "Mechanistic investigation of the catalytic hydrogenation of levulinic acid over Ru model catalyst surfaces" **Mamun O.**, Bond J.Q., Heyden A., AIChE annual meeting, San Francisco, CA, November 2016
5. "Theoretical investigation of the catalytic hydrodeoxygenation of levulinic acid over Ru(0001)" **Mamun O.**, Heyden A., SECS Annual Meeting, Asheville, NC, September 2016
6. "Mechanistic Investigation of the Aqueous Phase Hydrodeoxygenation of Levulinic Acid over Ru Catalysts," **Mamun O.**, A. Heyden, NAM, Denver, CO, June 2017.
7. "A delta learning approach to adsorption energy prediction on bimetallic alloy catalysts" **Mamun O.**, Boes J., Winther K., Bligaard T., ACS meeting, Orlando, FL, April 2019
8. "Catalysis-Hub.org: an open electronic structure database for surface reactions" Winther K. **Mamun O.**, Boes J., Bajdich M., Bligaard T., ACS meeting, Orlando, FL, April 2019

Software development projects

1. **CatKit**: A collaborative project where we developed a code to efficiently 1. enumerate the surface structures using graph theoretic approach, 2. automatic submission and curation of throughput jobs in various supercomputers, 3. machine learning fingerprint generator.
2. **CatLearn**: A collaborative project where we developed a machine learning code to perform regression, classification, fingerprint generation, feature reduction, GP guided optimization etc.
3. **CatHub**: A collaborative project where we developed a python API for our database Catalysis-Hub.org.
4. **Catalysis hub database** (www.catalysis-hub.org/profile/osman-mamun): Contributed over 85,000 surface reactions data to the database. All my codes used to generate the data and machine learning models can be found in https://github.com/mamunm/Bimetallic_Alloy_Codes
5. **ActiTOF**: An ongoing work on an active learning strategy for improving the accuracy of the TOF predictions based on all previous information, e.g., thermodynamic predictions, kinetic predictions, reconstruction predictions etc.
6. **Pswarm**: A side project where I'm developing an atomistic particle swarm optimizer for efficient optimization in high dimensional space.
7. **Data science**: In my free time, I'm trying to implement data science algorithms from scratch. Codes can be found here https://github.com/mamunm/data_dcience_algorithms

Skills

Programming language: Python, MATLAB, FORTRAN, C++

Quantum chemistry package: VASP, Quantum Espresso, TURBOMOLE, COSMO/COSMO-RS, MOPAC

Machine learning packages: scikit-learn, tensorflow, GPFlow, scikit-optimize, GPy

Machine learning algorithms: linear regression, logistic regression, clustering, classification, support vector machine, Gaussian Process, decision trees etc.

statistical techniques: f-test, t-test, hypothesis testing, ANOVA etc.

Numerical computing: Numpy, Scipy, Pandas

Relational Database: MySQL, sqlite3, postgresql

NoSQL Database: MongoDB

VCS: GIT, SVN