Salman Ahmad Khan

CONTACT INFORMATION

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APPOINTMENTS

Postdoctoral researcher, *Vlachos group*, Delaware Energy Institute, University of Delaware, Newark, DE, USA. (September 2021-Present)

EDUCATION

University of California, Santa Barbara

PhD in Chemical Engineering (September 2016-August 2021)

- GPA **3.97**/4.0

Indian Institute of Technology, Kanpur

B.tech in Chemical Engineering (May 2015)

- Cumulative Performance Index (CPI) of **8.9**/10

M.tech in Chemical Engineering (May 2016)

- Cumulative Performance Index (CPI) of **10.0**/10

TECHNICAL SKILLS

- **Languages:** Python, C/C++, FORTRAN
- **Software:** MATLAB, Mathematica, Gaussian, LAMMPS, VASP

RESEARCH INTERESTS

Molecular simulations, rare events methods, computational-catalysis, machine learning, population balance modeling, statistical hypothesis testing

RESEARCH EXPERIENCE

UD *Advisors: Prof. Dion Vlachos and Dr. Stavros Caratzoulas* **September 2021 - Present**

- **Rare events, global-optimization, and machine learning tools to model supported sub-nanometer metal clusters**: Developed actively trained ML potentials with basin-hopping to discover stable Al_2O_3 supported Pt clusters. Demonstrated that Pt/Al_2O_3 clusters show a 3D→2D transition with temperature using force bias monte carlo and umbrella sampling simulations. Results were confirmed with EXAFS experiments. Extended framework to model the effect of hydrogen adsorbates on Pt/Al_2O_3.
- **Effect of heteroatoms on catalyzing ethane dehydrogenation in chabazite supported Pt catalysts**: Computed ethane dehydrogenation free energies over metal substituted Pt/chabazite catalysts. Different types of metal (Ti, Sn, Hf, Zr) substituents and site-geometries were scanned and it was discovered that certain types of sites can lead to spin-crossing mechanisms.
- **Machine learning models to predict molecular properties**: Developing ML models to predict properties, such as viscosity, flash-point, toxicity of different types of molecules.
- **Statistical mechanics models for dynamically heated catalysts**: Developed an exactly solvable statistical mechanics model to study the behaviour of clusters under dynamic temperature control. Model was used to demonstrate stabilization of metastable cluster distributions with dynamic temperature pulsing.

UCSB *Advisors: Prof. Baron Peters and Prof. Susannah Scott* **September 2016 - August 2021**

- **Machine learning tools to model amorphous catalysts**: Developed machine learning, population balance modeling, and importance sampling tools to model the synthesis and activity of amorphous catalysts. Developed an amorphous catalyst model to demonstrate the efficiency of the developed methods against brute-force calculations.
- **Grafting $TiCl_4$ onto amorphous silica**: Modeled grafting kinetics of $TiCl_4$ onto amorphous silica using density functional theory parameterized population balance models. Model predictions were validated against EXAFS and IR measurements.
- **Inaccuracies/inefficiencies in infrequent metadynamics**: Demonstrated that hidden barriers in free energy surfaces can cause inaccuracies/inefficiencies in rates calculated using infrequent metadynamics (iMetaD). Demonstrated that umbrella sampling + dynamical correction methods are more robust and efficient than iMetaD.
- **Benchmarking atomistic models of amorphous silica**: Compared atomistic models of amorphous silica using statistical hypothesis testing methods (Kolmogorov Smirnov and Chi-squared tests). Developed probabilistic models to estimate the spatial distribution of silanols from EPR spectroscopy measurements. Validated existing atomistic amorphous silica models against experimentally determined parameters.

IIT Kanpur *Advisor: Prof. Raj Ganesh Pala* **August 2015 - April 2016**

- **Modeling vacancy-vacancy interactions on Ti doped ZnO**: Calculated vacancy migration barriers on Ti doped ZnO surfaces as a function of local vacancy concentration using the nudged elastic band method. Used calculations to explain experimentally observed hysteresis in CO oxidation over Ti doped ZnO catalysts.
- **Modeling Cyclic Voltammetry**: Developed C++ code to simulate cyclic voltammetry. Determined elementary hydrogen evolution reaction rate constants by fitting simulations to experimental rates.

Work Experience

Computational Modeling Intern, Whirlpool, Global Technology Engineering Center, Pune, India **May 2014 - July 2014**

Project supervisor: Mr.Nukul Sugandhi, Assistant Manager, Whirlpool

- Developed a mathematical model of condensation inside dishwashers and implemented it in MATLAB
- Determined parameters critical to water condensation and sticking on stainless steel surfaces
- Developed image processing tools to identify regions of maximum condensation on dishwasher walls
- Project awarded **2nd** prize out of 21 internee projects

Publications

$*$ indicates equal contribution and † indicates corresponding author

Published/Accepted/Under review

- Ricardo Pool-Mazun,* Vinson Liao,* **Salman A. Khan**,* Md Raian Yousuf, Abhijit Shrotri, Dionisios G. Vlachos,† Ayman M. Karim,† *Reversible Temperature-Induced Shape Transition of Pt Nanoparticles Supported on Al_2O_3*, under review, **ACS Nano**.

- **Salman A. Khan**, Stavros Caratzoulas, and Dionisios G. Vlachos,† *Catalyst cluster-induced support restructuring*, accepted **J. Phys. Chem. C.**, 2023. **(selected for supplementary cover)**
- Armin Shayesteh Zadeh, **Salman A. Khan**, Craig A. Vandervelden, and Baron Peters,† *Site-averaged ab initio kinetics: Importance learning for multistep reactions on amorphous supports*, **J. Chem. Theory Comput.**, 2023, 19, 10, 2873-2886.
- **Salman A. Khan**, Sahan Godahewa, Pubudu Wimalasiri, Ward Thompson, Susannah L. Scott, and Baron Peters,† *Grafting $TiCl_4$ onto amorphous silica: modeling effects of silanol heterogeneity*, **Chem. Mater.**, 2022, 34 (9), 3920–3930.
- Craig A. Vandervelden, **Salman A. Khan**, and Baron Peters,† *Importance learning estimator for the site-averaged turnover frequency of a disordered solid catalyst*, **J. Chem. Phys.**, 2020, 150 (24), 244120.
- **Salman A. Khan**, Bradley M. Dickson, Baron Peters,† *How fluxional reactants limit the accuracy/efficiency of infrequent metadynamics*, **J. Chem. Phys.**, 2020, 153 (5), 054125.
- Craig A. Vandervelden,* **Salman A. Khan**,* Susannah L. Scott, and Baron Peters,† *Site-averaged kinetics for catalysts on amorphous supports: an importance learning algorithm*, **React. Chem. Eng.**, 2020, 5 (1), 77-86.
- **Salman A. Khan**,* Craig A. Vandervelden,* Susannah L. Scott, and Baron Peters,† *Grafting metal complexes onto amorphous supports: from elementary steps to catalyst site populations via kernel regression*, **React. Chem. Eng.**, 2020, 5 (1), 66-76.

To be submitted (a copy of the manuscript can be provided upon request)

- **Salman A. Khan**, Susannah L. Scott, and Baron Peters,† *Statistical analysis of structural differences between computational models of silica*, to be submitted.
- Tarnuma Tabassum, **Salman A. Khan**, Baron Peters, Susannah L. Scott,† and Songi Han,† *EPR evidence for silanol clustering on silica surfaces*, to be submitted.

In preparation

- **Salman A. Khan***,† and Shikhar Misra,*,† *High-throughput screening of perovskite synthesis parameters from scientific literature with large language models*, in preparation.
- Hung-Ling Yu,* **Salman A. Khan**,* Dionisios G. Vlachos,† and Ayman Karim,† *Effect of temperature-induced cluster transformations on hydrogen adsorption on Alumina supported Pt clusters*, in preparation.
- **Salman A. Khan**, Dionisios G. Vlachos, and Stavros Caratzoulas,† *Effect of heteroatoms on catalyzing ethane dehydrogenation in chabazite supported Pt catalysts*, in preparation.
- George Yan,* **Salman A. Khan**,* and Dionisios G. Vlachos,† *Redox-Driven hydrogen adsorption and spillover at the Pt-γ-Alumina interface*, in preparation.
- Vinson Liao,* **Salman A. Khan**,* and Dionisios G. Vlachos,† *Stabilizing metastable particle distributions with dynamic temperature pulsing: insights from a simple model*, in preparation.

Invited Talks

- Statistical Thermodynamics & Molecular Simulations (STMS) Seminar Series, **2022**.
- Invited talk at the University of Kansas, Lawrence, KS, **2019**.

Conferences

- ACS Fall Meeting, San Francisco, CA, **2023** (**Future investigator spotlight oral presentation**).
- 28th North American Catalysis Meeting, Providence, RI, **2023** (**poster presentation**).
- DARWIN Computing Symposium, Newark, DE, **2023** (**poster presentation**).
- AIChE Annual Meeting, Phoenix, AZ, **2022** (**oral presentation**).
- ACS Fall Meeting, Chicago, IL, **2022** (**oral presentation**).
- AIChE Annual Meeting, Boston, MA, **2021** (**oral presentation**).
- CECAM Activated Events Online Conference, **2021** (**poster presentation**).
- AIChE Midwest Regional Conference, Chicago, IL, **2020** (**oral presentation**).
- AIChE Annual Meeting, Orlando, FL, **2019** (**oral presentation**).
- Summer school, Rare Events: Applications, Computation, and Theory, Indian Institute of Science, Bangalore, IN, **2019** (**participant**).
- Midwest Thermodynamics and Statistical Mechanics Conference, Urbana-Champaign, IL, **2019 (participant)**.
- Machine Learning in Science and Engineering, Atlanta, GA, **2019 (oral presentation)**.
- Spring Symposium of the Catalysis Club of Chicago, Chicago, IL, **2019** (**poster presentation**).
- 11th Annual Amgen-Clorox Graduate Student Symposium, UCSB, Santa Barbara, CA, **2018** (**poster presentation**).

Awards and Achievements

- Energy and Fuels Division (ENFL) **Future Investigator Spotlight** ACS Fall 2023 (2023).
- ACS 2022 talk selected for Sci-Mix poster session (upto 10 % talks selected from a division) (2022).
- Travel Award, Machine Learning in Science and Engineering Symposium, Atlanta (2019).
- **Academic Excellence** award 2015-16, IIT Kanpur, awarded to 2 students in the dual degree Chemical Engineering class (2016).
- **Academic Excellence** award 2013-14, IIT Kanpur, awarded to top 7% students in the institute (2015)
- Intern project at Whirlpool Corporation awarded the **2nd** prize out of 21 projects (2014).
- **Kishore Vaigyanik Protsahan Yojana (KVPY) scholarship**, offered by the Department Of Science and Technology India to around 500 students all over the country to pursue undergraduate studies in Physics, Chemistry, or Mathematics (2011) (declined).
- **Top 0.27%** in India in the Joint Entrance Examination conducted by the Indian Institutes of Technology (2011).

Service

- **Peer Review:** 28th North American Catalysis Society Meeting, MDPI Catalysts, MDPI Membranes, MDPI Processes, MDPI Molecules.
- Judge ACS Energy and Fuels Division graduate student poster session ACS Fall 2023.
- Session co-chair Multi-scale modeling AIChE 2023

Students Mentored

- Max Scizek: Modeling the distribution of active sites in multimetallic catalysts (2022-present).
- Jae Kim: Machine learning lubricant properties (2023-present).

Teaching Experience

- Developing animations on mathematical methods and reaction rate theory at youtube.com/@lipsum12
- Taught a class in Special Topics in Energy with Prof. Dion Vlachos, UD (2023)
- Reader, Advanced Theoretical Methods in Engineering, UCSB (2017)

- Teaching Assistant, Graduate Fluid Dynamics, IIT Kanpur (2016)
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