Armin Shayesteh Zadeh

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Education

University of Chicago, Chicago, IL
Postdoctoral Scholar, Advised by: A. L. Ferguson *June 2023 - Present*

University of Illinois at Urbana-Champaign, Urbana, IL
Ph.D. in Chemical and Biomolecular Engineering, Advised by: B. G. Peters *August 2018 - May 2023*

Sharif University of Technology, Tehran, Iran
B.Sc. in Chemical Engineering *September 2014 - June 2018*

Work Experience

University of Chicago June 2023 - Present

- **Postdoctoral Scholar**: advised by Dr. Andrew Ferguson, High-throughput virtual screening of protein catalyzed capture (PCC) agents for small molecule detection
  - Performing enhanced sampling molecular dynamics simulations to calculate the binding free energy of target and decoy molecules to PCC candidates and determining specificity and sensitivity.
  - Developing an active learning algorithm using multi-fidelity, multi-objective Bayesian optimization to search the PCC epitope sequence chemical space to find ideal candidates for binding to small molecule targets.

University of Illinois at Urbana-Champaign September 2018 - May 2023

- **Research assistant**: advised by Dr. Baron Peters, Multiscale modeling of complex chemical systems using first-principles, computational chemistry tools, and machine learning.
  - Developed an adaptive machine learning algorithm to efficiently and accurately estimate enthalpy distributions and highly active molecular structures from molecular dynamics simulations and density functional theory calculations.
  - Developed a multiscale model to quantitatively analyze the effects of conformer interconversion and dimerization reactions on the rate of crystal growth in the boundary layer and in an MSMPR crystallizer.
  - Developed a framework for studying the effects of diffusion limitations on the yield of reactions in series.
  - Developed a multiscale model for studying the two-step growth of amyloid fibrils validated with coarse-grained molecular dynamics simulations and experimental data.
- **Teaching assistant**:
  - **CHBE594AM Multiscale modeling**: Held discussion sessions for graduate and undergraduate level students on fundamentals of computational chemistry and instructed students on Python and scientific packages for performing density functional theory calculations and molecular dynamics simulations for reaction barrier calculations and structure optimization.
  - **CHBE441 Chemical reaction engineering**: Designed and implemented flipped classroom worksheets through the PrairieLearn platform and held discussion sessions for undergraduate students, covering fundamentals of chemical kinetics, reactor design, and catalysis.
  - **CHBE594BGP Chemical kinetics, catalysis, and reaction engineering**: Held discussion sessions for graduate students on advanced kinetics concepts including Markov processes, kMC-Gillespie algorithm (discrete stochastic variables), Fokker-Planck equation (continuous stochastic variables), as well as transition state theory and classical nucleation theory.

Publications

- **Site-averaged *ab initio* kinetics: Importance learning for multistep reactions on amorphous supports** *Journal of Chemical Theory and Computation*, 19, 10, 2873–2886 2023
  Developed an active learning algorithm that combines importance sampling and metric learning kernel regression to predict turnover frequencies for multistep reactions on single-atom catalysts supported on amorphous silica/silica-alumina using *ab initio* calculations.

- **On dimerization kinetics and boundary layer transport in crystal growth from dimers,** 2022
  Journal of Crystal Growth 601, 126913
  Extended the theoretical framework for studying the effects of conformational interconversion kinetics on crystal growth rate to dimerization reaction.
- **Crystal Growth Impedance from Slow Conformer Interconversion in Bulk Solution,** *Crystal Growth & Design* 22 (8), 4821-4827 2022
  Developed a theoretical framework to capture the effects of slow conformational interconversion kinetics on the population of crystals in an MSMPR reactor.
- **Conformational interconversion kinetics, boundary layer transport, and crystal growth impedance,** *Crystal Growth & Design* 22 (7), 4298-4304 2022
  Developed a theoretical framework to study the effects of conformational interconversion kinetics on the crystal growth rate near the crystal surface.
- **Multiscale Models for Fibril Formation: Rare Events Methods, Microkinetic Models, and Population Balances,** *Life* 11 (6), 570 2021
  Developed a micro-kinetic model, a coarse-grained representation, a custom force-field and molecular dynamics code with a Langevin integrator, and a population balance model for studying the growth of amyloid fibrils, as well as a model based on maximum likelihood estimation to estimate kinetic parameters from simulation or experimental data.
- **Secondary effectiveness factors for catalytic reactions in series: extension to slab, cylindrical, and spherical geometries,** *Reaction Chemistry & Engineering* 5 (10), 2003-2008 2020
  Developed secondary effectiveness factors for different pellet geometries to model the kinetics of diffusion-limited systems where $A \rightarrow B \rightarrow C$ reactions happen. Applied the secondary effectiveness factors to study the effect of catalyst properties on the selectivity of the intermediate product B.

Conference presentations

- "Secondary Effectiveness Factors for Catalytic Reactions in Series: A Unified Extension to Slab, Cylinder, and Spherical Geometries", **ACS Fall Meeting**, San Francisco, CA, August 2023
- "Crystal Growth Impedance from Boundary Layer Transport, Conformational Interconversion, and Dimerization Kinetics", **AIChE Annual Meeting**, Pheonix, AZ, November 2022
- "Crystal Growth Impedance from Boundary Layer Transport, Conformational Interconversion, and Dimerization Kinetics", **ChBE Graduate Research Symposium**, Urbana, IL, October 2022
- "Crystal Growth Impedance from Boundary Layer Transport, Conformational Interconversion, and Dimerization Kinetics", **ACS Fall Meeting**, Chicago, IL, August 2022
- "Secondary Effectiveness Factors for Catalytic Reactions in Series: A Unified Extension to Slab, Cylinder, and Spherical Geometries", **AIChE Annual Meeting**, Boston, MA, November 2021

Leadership and Honors

Honors and awards

- A.T. Widiger Summer Fellowship Award 2022
- ChBE Graduate Student Teaching Award 2021
- Iran's National Elites Foundation's Academic Excellence Award 2016-17
- Chemical Engineering Department Academic Achievement Award 2017

Volunteering

- **St. Elmo Brady Academy (SEBA) volunteer** 2021-23
  Student volunteer for providing project-learning opportunities in science, technology, engineering, and math for Booker T. Washington's students to address racial inequities in STEM fields.
- **ChBE GSAC student research symposium chair and social media coordinator** 2019-20
  Co-organizer of the annual graduate student research symposium for the chemical and bioengineering department and social media coordinator of GSAC for departmental and outreach events.
- **Sharif University's Farayand magazine and podcast editor, and social media coordinator** 2016-18
  Online content creator and editor for Farayand Scientific magazine's podcast and website.
- **Sharif Computer-aided Chemical Engineering Programming Contest (SC3) technical coordinator** 2017
  Organizer and coordinator for the chemical engineering department's SC3 competition.

SKILLS

- **Programming languages**: Python (proficient), MATLAB (proficient), C (intermediate), SQL (beginner), R (beginner)
- **Libraries/Technologies**: Tensorflow, PyTorch, Scikit-Learn, Numpy, Pandas, Jupyter, matplotlib, Seaborn, Plotly, ASE, BigQuery, Tableau, Excel/Sheets
- **Scientific Packages**: NAMD, Gaussian, ORCA, LAMMPS, Mathematica
- **Certifications**: Google data analyst(Coursera), DeepLearning.ai deep learning specialization(Coursera), DeepLearning.ai TensorFlow developer specialization(Coursera), DeepLearning.ai TensorFlow advanced techniques(Coursera)