# Mahdi Ghorbani

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## Education

- **PhD, Chemical and Biomolecular Engineering** — **University of Maryland College Park**
  *GPA: 3.92/4.0* — *Expected May 2022*
  ***Advisors:*** *Prof. Klauda, Dr. Brooks*
- **B.Sc, Chemical Engineering** — **University of Tehran**
  *GPA: 3.95/4.0* — *2012–2016*
  ***Advisor:*** *Dr. Salehi*

## Research Interests

- Computational protein engineering and design
- Geometrical deep learning
- Free energy calculations
- Computational structural biology
- Computational structure-based drug design
- Enhanced sampling methods

## Research Experience

- **Graduate Research Assistant** — University of Maryland, College Park, MD
  *Laboratory of Molecular and Thermodynamic Modeling* — *2018–Present*
  - **Permeability calculation using solubility diffusion models and MD simulations** Advisor: Prof. Klauda
  - **Investigating receptor binding and network analysis of spike protein in SARS-COV-2** Advisor: Prof. Klauda
  - **Computational study of small molecule drugs binding to PAS doamin of EAG channels** Advisor: Prof. Klauda
  - **Plexin dimerization in intracellular domain** Advisor: Prof. Klauda
  - **Conformational fluctuation of $\beta$2-microglobulin using deep learning and markov model** Advisor: Prof. Klauda
  - **Computational study of cell penetrating peptides interaction with membranes** Advisors: Prof. Klauda, Dr. Karlsson
  - **Deep generative language models and and molecular dynamics for antimicrobial peptide discovery** Advisors: Prof. Klauda, Dr. Karlsson
- **Pre-Doctoral IRTA Fellow** — National Institute of Health (NIH), Bethesda, MD
  *Laboratory of Computational Biology* — *2019–Present*
  - **Discovering allosteric pathway in GPCR using metadynamics and deep graph neural networks** Advisor: Dr. Brooks
  - **Modeling dynamics of protein folding using variational approach to markov processes and graph neural networks (GraphVAMPNet)** Advisor: Dr. Brooks
  - **Gaussian mixture variational autoencoder for dimensionality reduction and clustering of protein folding simulations** Advisor: Dr. Brooks
  - **Host-guest binding free energy calculations with Replica Exchange Umbrell Sampling (REUS)** Advisor: Dr. Brooks
- **Undergraduate Research Assistant** — University of Tehran, Tehran, Iran
  *Chemical Engineering Department* — *2015–2017*
  - **Investigating the electrocatalytic properties of Graphene based catalysts for PEM Fuel Cell application** Advisor: Prof. Khodadadi
  - **Graphene oxide and Graphene Quantum Dots for drug delivery of Tamoxifen and Curcumin** Advisor: Dr. Salehi

## Publications

- **Ghorbani, M.**, Prasad S., Klauda, J. B; Brooks, B. R. **"GraphVAMPNet, using graph neural networks and variational approach to markov processes for dynamical modeling of biomolecules."** *J. Chem. Phys.* (2022, submitted) arXiv preprint arXiv:2201.04609
- **Ghorbani, M.**; Prasad, S.; Klauda, J. B.; Brooks, B. R. **Variational Embedding of Protein Folding Simulations Using Gaussian Mixture Variational Autoencoders.** The Journal of Chemical Physics 2021, 155 (19), 194108.
- **Ghorbani, M.**; Hudson, P. S.; Jones, M. R.; Aviat, F.; Meana-Pañeda, R.; Klauda, J. B.; Brooks, B. R. **A Replica Exchange Umbrella Sampling (REUS) Approach to Predict Host–Guest Binding Free Energies in sampl8 Challenge.** Journal of Computer-Aided Molecular Design 2021, 35 (5), 667–677.
- **Ghorbani, M.**; Brooks, B. R.; Klauda, J. B. **Exploring Dynamics and Network Analysis of Spike Glycoprotein of SARS-COV-2.** Biophysical Journal 2021, 120 (14), 2902–2913.

- **Ghorbani, M.**; Brooks, B. R.; Klauda, J. B. **Critical Sequence Hotspots for Binding of Novel Coronavirus to Angiotensin Converter Enzyme as Evaluated by Molecular Simulations.** The Journal of Physical Chemistry B 2020, 124 (45), 10034–10047.
- **Ghorbani, M.**; Wang, E.; Krämer, A.; Klauda, J. B. **Molecular Dynamics Simulations of Ethanol Permeation through Single and Double-Lipid Bilayers.** The Journal of Chemical Physics 2020, 153 (12), 125101.
- Nikfarjam, S., **Ghorbani, M.**, Adhikari, S., Karlsson, A. J., Jouravleva, E. V., Woehl, T. J., Anisimov, M. A. (2019). **Irreversible Nature of Mesoscopic Aggregates in Lysozyme Solutions.** Colloid Journal, 81(5), 546-554.

## Talks and Presentations

- **Ghorbani M. "Unraveling the allosteric activation of GPCRs using Metadynamics and deep learning"** Conference talk, BPS2022, San Francisco, US
- **Ghorbani M. "Dynamical coarse graining of molecular systems using GraphVAMPNets"** LCB seminar series, 2021, NIH, Bethesda
- **Ghorbani M.; Brooks B. R.; Klauda J. B.; "An integrative MD simulation and network analysis approach to study Glycosylation of spike in SARS-COV-2"** Virtual Poster Presentation, BPS2021
- **Ghorbani M. "Gausisan mixture variational autoencoders for dimensionality reduction and clustering of protein folding simulations"** LCB seminar series, 2020, NIH, Bethesda
- **Ghorbani M. "Investingating dynamics and network analysis of spike protein in SARS-COV-2"** LCB seminar series, 2020, NIH
- **Ghorbani M., Harron M., Wang E., Klauda J. B., "Mechanism of permeability and toxicity of alcohols to cell membranes by MD simulations"** Poster Presentation ACS2019, San Diego, US
- **Ghorbani M., Wang E., Klauda J. B., "Calculating Ethanol Permeability of Membranes Through Molecular Dynamics Simulations"** Poster Presentation BPS2019, Baltimore, US

## Honors and Awards

- Outstanding Teaching Assistant - October, 2019
- Anton2 Award, Pittsburgh Super-computing center - 2019,2020
- University of Maryland Dean's Fellowship Award - August, 2017
- Among top five students of Chemical Engineering in University of Tehran - 2012-2016
- Ranked top 10 in $4^{th}$ and $5^{th}$ National Nanotechnology competition, Tehran Iran - 2014,2015

## Other Academic Activities

- **President of Chemical And Biomolecular Graduate Student Association (CGA)** University of Maryland
  *Professional events for graduate students.* *2019–2021*
- **Graduate Teaching Assistant** University of Maryland
  *Thermodynamics I* *Fall 2018*
- **Graduate Teaching Assistant** University of Maryland
  *Thermodynamics II* *Spring 2019*
- **Undergraduate Teaching Assistant** University of Tehran
  *Application of Computational techniques in Chemical Engineering* *2015–2017*