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, Prof. 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
- Enhanced sampling methods

Research Experience

- **Graduate Research Assistant** — University of Maryland, College Park
  Laboratory of Molecular Dynamics Simulations — *January 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 β2-microglobulin using deep learning and markov model** Advisor: Prof. Klauda
  - **Computational study of cell penetrating peptides interaction with membranes** Advisors: Prof. Klauda, Dr. Karlsson

- **Pre-Doctral IRTA Fellow** — National Institute of Health (NIH)
  Computational Biophysics group — *since 2019*
  - **Discovering allosteric pathway in GPCR using metadynamics and deep graph neural networks** Advisor: Prof. Brooks
  - **modeling dynamics of protein folding using variational approach to markov processes and graph neural networks (GraphVAMPNet)** Advisor: Prof. Brooks
  - **Gaussian mixture variational autoencoder for dimensionality reduction and clustering of protein folding simulations** Advisor: Prof. Brooks
  - **Host-guest binding free energy calculations with Replica Exchange Umbrell Sampling (REUS)** Advisor: Prof. Brooks

- **Undergraduate research assistant** — University of Tehran
  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, Mahdi**, et al. **"GraphVAMPNet, using graph neural networks and variational approach to markov processes for dynamical modeling of biomolecules."** arXiv preprint arXiv:2201.04609 (2022)
- **Ghorbani, Mahdi**, et al. **"Variational embedding of protein folding simulations using Gaussian mixture variational autoencoders."** The Journal of Chemical Physics 155.19 (2021): 194108.
- **Ghorbani, Mahdi**, et al. **"A replica exchange umbrella sampling (REUS) approach to predict host–guest binding free energies in SAMPL8 challenge."** Journal of computer-aided molecular design 35.5 (2021): 667-677.
- **Ghorbani, Mahdi**, Bernard R. Brooks, and Jeffery B. Klauda. **"Exploring dynamics and network analysis of spike glycoprotein of SARS-COV-2."** Biophysical Journal (2021)
- **Ghorbani, Mahdi**, Bernard R. Brooks, and Jeffery B. Klauda. **"Critical sequence hotspots for binding of novel coronavirus to angiotensin converter enzyme as evaluated by molecular simulations."** The Journal of Physical Chemistry B 124.45 (2020): 10034-10047
- **Ghorbani, Mahdi**, et al. **"Molecular dynamics simulations of ethanol permeation through single and double-lipid bilayers."** The Journal of Chemical Physics 153.12 (2020): 125101.

Talks and Presentations

- **M, Ghorbani, B. R. Brooks, J. B. Klauda, "An integrative MD simulation and network analysis approach to study Glycosylation of spike in SARS-COV-2"** Virtual Poster Presentation, BPS2021
- **M. Ghorbani, M. Harron, E. Wang, J. B. Klauda, "Mechanism of permeability and toxicity of alcohols to cell membranes by MD simulations"** Poster Presentation ACS2019, San Diego, US
- **M. Ghorbani, E Wang, J. B. Klauda "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*