

# Mahdi Ghorbani

website: ghorbanimahdi73.github.io

Linkedin: Mahdi-Ghorbani

Email: ghorbani.mahdi73@gmail.com

Mobile: +1-202-867-4131

## EDUCATION

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- **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

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- Computational protein engineering and design
  - Geometrical deep learning
  - Free energy calculations
  - Enhanced sampling methods

## RESEARCH EXPERIENCE

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- **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
    - Plexin dimerization in intracellular domain Advisor: Prof. Klauda
    - Conformational fluctuation of  $\beta$ 2-microglobulin using deep learning and markov model Advisor: Prof. Klauda
    - Engineering cell penetrating peptides for cargo delivery into cells Advisors: Prof. Klauda, Dr. Karlsson
  - **Pre-Doctoral IRTA Fellow** National Institute of Health (NIH)  
Computational Biophysics group since 2019
    - Gaussian mixture variational autoencoder for dimensionality reduction and clustering of protein folding simulations Advisor: Prof. Brooks
    - Modeling dynamics of protein folding using GraphVAMPNet Advisor: Prof. Brooks
    - Neural relational inference and metadynamics for allostery in GPCR 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

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- 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

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- 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

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- 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<sup>th</sup> and 5<sup>th</sup> National Nanotechnology competition, Tehran Iran - 2014,2015

## OTHER ACADEMIC ACTIVITIES

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- **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