Rezvan Shahoei

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Education

Ph.D., Physics   **May 2020**

University of Illinois at Urbana-Champaign (UIUC)

Thesis Title: Computational Modeling and Simulation of Ligand-Gated Ion Channels

M.Sc., Physics   **July 2010**

Sharif University of Technology, Iran

Thesis Title: Abelian Sandpile Models and Surface Growth

B.Sc., Physics   **July 2008**

University of Tehran, Iran

Software and Programming Skills

- Online Course Certificates: Applied Machine Learning: Foundations (LinkedIn Learning), Applied Machine Learning: Algorithms (LinkedIn Learning)

- Python, shell scripting, Tcl, LaTeX, version control (CVS and Git)

- Running jobs on CPU/GPU clusters, supercomputers (Blue Waters, Stampede, and Bridges), and NVIDIA DGX-2

- Molecular dynamics software (NAMD and VMD), computational biology and chemistry software (Chimera, Gaussian, MOE, and PyMOL)

Experience

Research Assistant at the Theoretical and Computational Biophysics Group at UIUC   **May 2012–December 2019**

- Built multi-million atom models of biological systems and performed equilibrium and non-equilibrium molecular dynamics (MD) simulations on CPU/GPU clusters, supercomputers, and NVIDIA DGX-2

- Implemented enhanced sampling techniques, free energy calculation methods (FEP and umbrella sampling), and docking in small molecule-protein studies

- Analyzed hundreds of gigabytes of MD trajectories using VMD, and made demos and videos of microsecond-long MD trajectories of complex biomolecular systems

- Analyzed data and generated figures for publications using Python (SciPy, pandas, and Matplotlib)

- Collaborated with multiple experimental groups and validated experimental results using various computational methods

- Participated in writing several NIH and NSF proposals for funding and supercomputing allocations at the NIH Center for Macromolecular Modeling and Bioinformatics by contributing material and coordinating inputs from teams of scientists and software developers

- Was in charge of the highlights and announcements sections of the NIH Center for Macromolecular Modeling and Bioinformatics website

Teaching Assistant at the Department of Physics at UIUC   **August 2010–May 2018**

- Courses taught: Non-equilibrium Statistical Mechanics, Thermal & Statistical Physics, Relativity & Math Applications, Mechanics & Heat

- Created material, led discussion sessions, and assessed students' performance for undergraduate courses

- Earned the Graduate Teacher Certificate demonstrating advanced professional communication and instructional skills

Publications

- **R. Shahoei** and E. Tajkhorshid (2020) Menthol binding to the human α4β2 nicotinic acetylcholine receptor, facilitated by its strong partitioning in membrane. *J. Phys. Chem. B*, 124(10): 1866–1880
- B. J. Henderson, S. Grant, B. W. Chu, **R. Shahoei**, S. M. Huard, S. S. M. Saladi, E. Tajkhorshid, D. A. Dougherty, and H. A. Lester (2018) Menthol stereoisomers exhibit different effects on α4β2 nAChR upregulation and dopamine neuron spontaneous firing. *eNeuro*, 5(6). pii: ENEURO.0465-18.2018
- Chakravarti, K. Selvadurai, **R. Shahoei**, H. Lee, S. Fatma, E. Tajkhorshid, and R. Huang (2018) Reconstitution and substrate specificity of the antiviral radical SAM enzyme viperin. *J. Biol. Chem.*, 293(36): 14122–14133
- S. Maji, **R. Shahoei**, K. Schulten, and J. Frank (2017) Quantitative Characterization of Domain Motions in Molecular Machines. *J. Phys. Chem. B*, 121(15): 3747–3756

Presentations

- Menthol binds to extracellular and transmembrane domains of the human α4β2 nicotinic receptor. 63rd Annual Meeting of the Biophysical Society, Baltimore (March 2019)

- Menthol's interaction with membrane and human nicotinic receptor. CPLC/CBQB Graduate Student and Postdoc Symposium, UIUC (April 2018)

- Structure and function of YidC. Physics of Living Systems Student Research Network, University of Maryland (July 2015)

Awards

- Graduate College Firdawsi Science Fellowship Award, UIUC (2018–2019)

- Engineering College Mavis Fellowship, UIUC (2017–2018)

- Department of Physics Graduate Student Travel Award, UIUC (Spring 2015 & 2019)

- University Fellowship, Department of Physics, UIUC (Spring 2014)

- University Fellowship for Excellence in Teaching Undergraduate Courses, UIUC (2012)

- Department of Physics Scott Anderson Award for Outstanding Teaching, UIUC (2011)