# Aliasghar Sepehri

Oden Institute for Computational Engineering and Sciences, The University of Texas at Austin

201 E 24th St, Austin, TX 78712

Cell Phone: 225-773-9208

Email: aliasghar.sepehri@austin.utexas.edu

Green Card holder

## EXPERIENCE

**Research Fellow:** Oden Institute for Computational Engineering and Sciences, The University of Texas at Austin, Austin, TX September 2022 - Now

Advisor: Prof. Ron Elber

**Postdoctoral Research Associate:** Department of Chemistry and Biochemistry, The City College of New York, New York, NY July 2018 – August 2022

Advisor: Prof. Themis Lazaridis

## EDUCATION

**PhD**: Chemistry-Physical Chemistry (GPA 3.67/4.0) Fall 2012 – Spring 2018

Department of Chemistry, Louisiana State University, Baton Rouge, LA

Dissertation: “Innovative Monte Carlo Methods for Sampling Molecular Conformations”

Advisor: Prof. Bin Chen

**MS**: Chemical Engineering-Nanotechnology (GPA 3.85/4.0) Fall 2007 – Spring 2010

Department of Chemical Engineering, Amirkabir University of Technology, Tehran, Iran

Thesis: “A study on liquid formation from vapor from nanostructural view”

Advisor: Prof. Hamid Modarress

**BS**: Chemical Engineering-Petro Chemistry (GPA 3.46/4.0)  Fall 2002 – Spring 2007

Department of Chemical Engineering, Amirkabir University of Technology, Tehran, Iran

Advisor: Prof. Hamid Modarress

**Highlighted MS. and PhD. Coursework**: Quantum Chemistry, Computational Chemistry, Statistical Thermodynamics, Molecular Simulation Methods, Mathematical Methods in Chemistry, Numerical Methods, Physical Spectroscopy, Advanced Thermodynamics

## RESEARCH INTEREST

1. Molecular dynamics simulation of antimicrobial peptides

2. Free energy calculation

3. Development of new implicit models for peptide-membrane simulation

4. Development of new Monte Carlo methods for sampling molecular conformations and molecular transfer between phases

5. Molecular dynamics simulation of phase separation

6. Multicomponent and Ion-induced nucleation in atmosphere

7. Computational chemistry calculations (DFT, HF, etc.)

## COMPUTER SKILLS

Programming: FORTRAN, MATLAB, Python, Tcl, shell script

Applications: LAMMPS, CHARMM, NAMD, GROMACS, VMD, Towhee (Monte Carlo), Gaussian, PyMOL

Operating systems: Windows, LINUX

# TEACHING

1. Physical Chemistry 3493 Lab Fall 2012, Spring 2013

2. Physical Chemistry 3491, Grading and Recitation Fall 2014, 2015, 2016

3. General Chemistry 1212 Lab Fall 2015, 2016, 2017 Spring 2016, 2018

# PUBLICATIONS

**Sepehri, A.**; Amjad-Iranagh, S.; Golzar, K.; Modarress, H., Homogeneous and heterogeneous nucleation of water vapor: A comparison using molecular dynamics simulation. *Chem. Phys.* **2013,** *423*, 135-141.

**Sepehri, A.**; Loeffler, T. D.; Chen, B., Improving the efficiency of configurational-bias Monte Carlo: A density-guided method for generating bending angle trials for linear and branched molecules. *J. Chem. Phys.* **2014,** *141* (7), 074102.

Loeffler, T. D.; **Sepehri, A.**; Chen, B., Improved Monte Carlo Scheme for Efficient Particle Transfer in Heterogeneous Systems in the Grand Canonical Ensemble: Application to Vapor–Liquid Nucleation. *J. Chem. Theory Comput.* **2015,** *11* (9), 4023-4032.

**Sepehri, A.**; Loeffler, T. D.; Chen, B., Improving the efficiency of configurational-bias Monte Carlo: A Jacobian-Gaussian scheme for generating bending angle trials for linear and branched molecules. *J. Chem. Theory Comput.* **2017,** *13* (4), 1577-1583.

**Sepehri, A.**; Loeffler, T. D.; Chen, B., Improving the efficiency of configurational-bias Monte Carlo: Extension of the Jacobian-Gaussian scheme to interior sections of cyclic and polymeric molecules. *J. Chem. Theory Comput.* **2017,** *13* (9), 4043-4053.

Zahraeifard, S.; Foroozani, M.; **Sepehri, A.**; Oh, D.; Wang, G.; Mangu, V.; Chen, B.; Baisakh, N.; Dassanayake, M.; Smith, A., H2A.Z regulates transcriptional responses to

nutrient deprivation in accordance with genic location and gene function. *Journal of Experimental Botany*. **2018,** *69* (20), 4907-4919.

Ogunronbi, K.; **Sepehri, A.**; Chen, B.; Wyslouzil, B., Vapor phase nucleation of the short-chain n-alkanes (n-pentane, n-hexane and n-heptane): Experiments and Monte Carlo simulations. *J. Chem. Phys*. **2018,** *148* (14), 144312. (***Selected as a 2018 Editors' Choice article***)

**Sepehri, A.**; PeBenito, L.; Pino-Angeles, A.; Lazaridis, T., What Makes a Good Pore Former: A Study of Synthetic Melittin Derivatives. *Biophysical Journal.* **2020,** *118* (8), 1901-1913.

Nepal, B.; **Sepehri, A.**; Lazaridis, T., Mechanisms of negative membrane curvature sensing and generation by ESCRT III subunit Snf7. *Protein Science.* **2020,** *29* (6), 1473-1485.

**Sepehri, A.**; Nepal, B.; Lazaridis, T., Lipid interactions of an actinoporin pore-forming oligomer. *Biophysical Journal.* **2021,** *120* (8), 1357-1366.

**Sepehri, A.**; Nepal, B.; Lazaridis, T., Distinct modes of action of IAPP oligomers on membranes. *J. Chem. Inf. Model.* **2021,** *61* (9), 4645-4655.

Nepal, B.; **Sepehri, A.**; Lazaridis, T., Mechanism of negative membrane curvature generation by I-BAR domains. *Structure.* **2021,** *29* (12), 1440-1452. e4.

Lazaridis, T.; **Sepehri, A.**, Amino acid deprotonation rates from classical force fields. *J. Chem. Phys*. **2022,** *157* (8), 085101.

**Sepehri, A.**; Lazaridis, T., Putative Structures of Membrane-Embedded Amyloid β Oligomers. *ACS Chem. Neurosci.* **2023,** *14* (1), 99-110.

# ORAL PRESENTATION

**Sepehri, A.**; Loeffler, T. D.; Chen, B., Configurational bias Monte Carlo: Bending angle generation. Physical Chemistry seminar, Department of Chemistry, LSU, Baton Rouge, LA (Fall 2013)

**Sepehri, A.**; Loeffler, T. D.; Chen, B., Improvement in Configurational bias Monte Carlo. Physical Chemistry seminar, Department of Chemistry, LSU, Baton Rouge, LA (Fall 2014)

**Sepehri, A.**; Loeffler, T. D.; Chen, B., Improvement in Fixed Endpoints Configurational bias Monte Carlo. Physical Chemistry seminar, Department of Chemistry, LSU, Baton Rouge, LA (Fall 2015)

**Sepehri, A.**; Loeffler, T. D.; Chen, B., The effect of ammonia and amines in atmospheric nucleation. Physical Chemistry seminar, Department of Chemistry, LSU, Baton Rouge, LA (Fall 2016)

**Sepehri, A.**; Chen, B., A Jacobian-Gaussian method for efficient exploration of conformational space. Southeastern Theoretical Chemistry Association Meeting (SETCA), Baton Rouge, LA (May 2018)

**Sepehri, A**, Advanced Monte Carlo methods for sampling molecular conformations and nucleation. The City College of New York, New York, NY (May 2018)

**Sepehri, A.**; PeBenito, L.; Pino-Angeles, A; Lazaridis, T, What makes a good pore forming peptide. The City College of New York, New York, NY (Dec 2019)

# POSTER PRESENTATIONS

**Sepehri, A.**; Loeffler, T. D.; Chen, B., A Density-guided Method for Improving Conformational Sampling of Linear, Branched and Cyclic Molecules. 250$^{th}$ ACS National Meeting, Boston, MA (Fall 2015)

Loeffler, T. D.; **Sepehri, A.**; Chen, B., Monte Carlo method development and application towards nucleation studies. Graduate Student Poster Competition, Department of Chemistry, LSU, Baton Rouge, LA (Spring 2014)

Loeffler, T. D.; **Sepehri, A.**; Chen, B., Monte Carlo method development and application towards nucleation studies. Graduate Student Poster Competition, Department of Chemistry, LSU, Baton Rouge, LA (Spring 2015)

**Sepehri, A.**; PeBenito, L.; Pino-Angeles, A; Lazaridis, T, Membrane pore formation by melittin derivatives. 64th Annual Meeting of the Biophysical Society, San Diego, CA (Feb 2020)

## NATIONAL SOCIETIES

Member of American Chemical Society (ACS), 2015-present

Member of Biophysical Society, 2019-present

## CONFERENCE ATTENDED

250th ACS National Meeting, Boston, MA (August 2015)

Southeastern Theoretical Chemistry Association Meeting (SETCA), Baton Rouge, LA (May 2018)

63rd Annual Meeting of The Biophysical Society (BPS), Baltimore, MD (March 2019)

64th Annual Meeting of The Biophysical Society (BPS), San Diego, CA (Feb 2020)

## AWARDS AND HONORS

Research Assistant Scholar Award 2016-17, Department of Chemistry, LSU

Neil Kestner Physical Chemistry Graduate Student Award 2016-17, Department of Chemistry, LSU

## REFERENCES

Prof. Themis Lazaridis, Department of Chemistry and Biochemistry, The City College of New York, New York, NY, USA

Email: tlazaridis@ccny.cuny.edu

Contact: 212-650-8364

Prof. Bin Chen, Department of Chemistry, Louisiana State University, Baton Rouge, LA, USA

Email: binchen@lsu.edu

Contact: 225-578-4094

Prof. Kenneth Lopata, Department of Chemistry, Louisiana State University, Baton Rouge, LA, USA

Email: klopata@lsu.edu

Contact: 225-578-2063

Prof. Daniel Kuroda, Department of Chemistry, Louisiana State University, Baton Rouge, LA, USA

Email: dkuroda@lsu.edu

Contact: 225-578-1780

Prof. Dorel Moldovan, Department of Mechanical & Industrial Engineering, Louisiana State University, Baton Rouge, LA, USA

Email: dmoldo1@lsu.edu

Contact: 225-578-6488

Prof. Revati Kumar, Department of Chemistry, Louisiana State University, Baton Rouge, LA, USA

Email: revatik@lsu.edu

Contact: 225-578-0907