Leila Tohidifar

Curriculum Vitae

***Gender*:** Female

***Date of Birth*:** 29 January 1986

Nationality: Iranian

***Marital Status*:** Single

***Language*:** Persian, English

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***Email*:** Leila.tohidifar@modares.ac.ir, l.tohidifar@gmail.com

Education

(2014-2020)

Ph.D. in Physical Chemistry at Faculty of Sciences, Department of Chemistry, Tarbiat Modares University, Tehran, Iran.

***Thesis Title*:** Investigation of Some Drugs Interactions with Carbon Nanotubes Functionalized with PW3 Peptide: A Molecular Dynamics Simulation Study

***Supervisor*:** Prof. Dr. Nasser L. Hadipour

(07/2018-01/2019)

Visiting PhD student at the Computational Biochemistry group at Institute of Biological Information Processing: Structural Biochemistry (IBI-7), Forschungszentrum Jülich, **Germany**.

***Project Title*:** Investigation of Anticancer Drug Interactions with PW3 Peptide Functionalized Carbon Nanotube and Cell Membrane

***Supervisor*:** Prof. Dr. Birgit Strodel

(2012-2014)

M.Sc. in physical chemistry at Institute for Advanced Studies in Basic Sciences (IASBS), Zanjan, Iran.

***Thesis Title*:** Nano-scale Structural Organization, Thermodynamics, and Dynamics of the Ionic Liquid 1-hexyl-2,3-dimethylimidazolium bis(fluorosulfonyl)imide and Its Mixture with Acetonitrile: A Molecular Dynamics Simulation Study

***Supervisor*:** Dr. Mohammad. H Kowsari

(2005-2009)

BSc in pure chemistry at Payame Noor University, Zanjan, Iran.

Awards

- **(July 2018 - January 2019)**

  Fellowship of the Ministry of Science, Research and Technology of Iran.

- **(November 2018 - January 2019)**

  Fellowship of the German Academic Exchange Service (**DAAD**) via the German-Iranian Scholarship Program (GISP).

- **Teaching Qualification Certificate** received from Tarbiat Modares University

Research Interests

1. Molecular dynamics (MD) simulation study of biomolecules, proteins, drugs, nanotubes, and cell membranes and investigation of their interactions such as protein-protein, protein-nanotube and protein-lipid.

2. Molecular Dynamics (MD) Simulation of ionic liquids with the aim of investigating the microscopic structure, dynamics, transport, and thermodynamic properties of these neoteric green solvents in the pure and/or mixture form.

Publications

1. Tohidifar, L., Strodel, B. (2021). Molecular Dynamics Studies for Enhancing the Anticancer Drug Efficacy: Towards Designing a New Carbon Nanotube-Based Paclitaxel Delivery Systems. *J. Mol. Liq*, *323*, Article 114386. https://doi.org/10.1016/j.molliq.2020.114638

2. Tohidifar, L., L. Hadipour., N. (2019). Tracing Chirality, Diameter Dependence, and Temperature-Controlling of Single-Walled Carbon Nanotube Non-Covalent Functionalization by Biologically Compatible Peptide: Insights from Molecular Dynamics Simulations. *J Mol Model*, *25*(9), 274-288. https://doi.org/10.1007/s00894-019-4154-9

3. Kowsari., M. H., Tohidifar., L. (2018). Systematic Evaluation and Refinement of Existing All-Atom Force Fields for the Simulation of Liquid Acetonitrile. *J. Comput. Chem.*, *39*(23), 1843-1853. https://doi.org/10.1002/jcc.25337

The Cover Image related to this paper published on issue 23, vol. 39, 24 September 2018, on *J. Comput. Chem.*

4. Kowsari., M. H., Tohidifar., L. (2016). Tracing Dynamics, Self-Diffusion, and Nanoscale Structural Heterogeneity of Pure and Binary Mixtures of Ionic Liquid 1-Hexyl-2,3-dimethylimidazolium Bis(fluorosulfonyl)imide with Acetonitrile: Insights from Molecular Dynamics Simulations. *J. Phys. Chem. B*, 120(41), 10824-10838. https://doi.org/10.1021/acs.jpcb.6b08396

Manuscript in Progress

Leila Tohidifar, Birgit Strodel

Title: "Improving Delivery and Cellular Diffusion of Paclitaxel Using Peptide Functionalized Single-Walled Carbon Nanotube: Insights from Molecular Dynamics Simulations"

Conferences

1. L. Tohidifar, N. L. Hadipour, "Preparation of Water Soluble Single Walled Carbon Nanotubes: Study of the Chirality Effect Insights from Molecular Dynamics Simulations", *The 22nd Iranian Physical Chemistry Conference (IPCC)*, University of Zanjan, Zanjan, Iran, (2019).

2. L. Tohidifar, N. L. Hadipour, "Molecular Dynamics Study of pH-Dependent PW3 Peptide Modification of Single-Walled Carbon Nanotube", *The 21st Iranian Physical Chemistry Conference (IPCC)*, Azarbaijan Shahid Madani University, Tabriz, Iran, (2018).

3. L. Tohidifar, N. L. Hadipour, "Molecular Dynamics Simulations for Optimization of Functionalizing the Single-Walled Carbon Nanotubes by PW3 Peptide", *The 3rd Conferences on Protein & Peptide Sciences*, Shiraz University, Shiraz, Iran, (2018).

4. **L. Tohidifar, N. L. Hadipour,** "On the Carbon Nanotubes as Novel Candidates for Drug Delivery Systems: A Review of Latest Progresses and Achievements", *5th International Conference of Young Scientists (Chemistry Today-2016)*, Agricultural University of Georgia, Tbilisi, Georgia, 20-22, (2016).

5. **M. H. Kowsari, L. Tohidifar,** "Molecular Dynamic Simulation Study of the Nano-scale Segregated Structure of Ionic Liquid 1-Hexyl-2,3-dimethylimidazolium Bis(fluorosulfonyl)imide and Its Mixture with Acetonitrile", *The 2nd National Congress and Workshops on Nanoscience & Nanotechnology (NCWNN)*, Kharazmi University, Tehran, Iran, 1-4, (2015).

6. **M. H. Kowsari, L. Tohidifar,** "A Thermodynamic Study of the Ionic Liquid 1-Hexyl-2,3-dimethyl-imidazolium Bis(fluorosulfonyl)imide and Its Mixture with Acetonitrile Using Molecular Dynamics Simulation ", *The 2nd Regional Conference on Climate Change & Global Warming, IASBS*, Zanjan, Iran , p18-1-p18-6, (2014).

7. **M. H. Kowsari, L. Tohidifar,** "Effect of Adding Acetonitrile on the Dynamic Properties of 1-Hexyl-2,3-dimethylimidazolium Bis(flourosulfonyl)imide ([hmmim][FSI]) Ionic Liquid", *Proceeding of the 17th Iranian Physical Chemistry Conference (IPCC)*, K. N. Toosi University, Tehran, Iran, 1091-1093, (2014).

Participant in Workshops

1. The Online workshop on "**The application of Gaussian and Hyperchem Softwares in Computational Chemistry**", *Iran Nanotchnology Innovation Council*, Iran, October (**2020**). Received the highest score among all participates (100 out of 100).

2. The academic Online workshop on "**Advanced Course of Molecular Dynamics Simulation Using the NAMD and VMD packages (Simulation of Cell Membrane Proteins and Free Energy Calculations**", *Iran Nanotchnology Innovation Council*, Iran, September (**2020**). Received the highest score among all participates (100 out of 100).

3. The Online workshop on "**Molecular Dynamics Simulation Using the NAMD package**", *Iran Nanotchnology Innovation Council*, Iran, June (**2020**). Received the highest score among all participates (91 out of 100).

4. The academic workshop on "**Simulation of Cell Membrane Proteins**", Institute of Biochemistry and Biophysics, *University of Tehran*, Tehran, Iran, June (**2017**).

5. The academic workshop on "**Simulation of Nano-Structures Using the COMSOL Software**", *Kharazmi University*, Tehran, Iran, May (**2015**).

6. The academic workshop on "**Gaussian Software and Its Application in Pharmaceutical Compounds**", *Kharazmi University*, Tehran, Iran, May (**2015**).

Teaching in Workshop

Teaching of molecular dynamics simulation using the GROMACS package at the workshop on "**GROMACS Package and Its Application in the Study of Interactions of Drug Delivery Systems and Cell Membranes**", *22nd Iranian Physical Chemistry Conference (IPCC)*, University of Zanjan, Zanjan, Iran, August (**2019**).

Computer Skills

1. Working with the Linux operating system environments and multiprocessor clusters, familiar with installation of programs in Linux machines.

2. Classical molecular dynamics simulations of various systems with the available simulation packages such as **DL_POLY**, **NAMD**, and **GROMACS**.

3. Work ability with various simulation input generators and analysis programs such as **CHARMMGUI**, **VMD**, **Packmol**, **PyMOL**, **Hyperchem, Molden**, **Mercury**, **Material Studio**, **Travis** and **Rasmol.**

4. Some experiences in using the **Gaussian 03/09** suite of programs and **AMBER** code for optimization of structures and extracting the atomic partial charges and force field parameters necessary for MD simulations.