Leila Lotfikatooli
+98(911)175-0546 | l.lotfi@gu.ac.ir
Golestan University, Gorgan, Golestan, Iran

Education

PhD., Chemical Engineering, Ferdowsi University of Mashhad, Mashhad, Iran, 2013-2017
Dissertation: "Prediction of Adsorption Isotherms via Molecular Simulation and Global Optimization"
B.Sc., Mechanical Engineering, Azad university. Iran, 2012-2015
MSc., Chemical Engineering, Iran University of Science and Technology, Tehran, Iran, 2009-2011
B.Sc, Chemical Engineering, Amir Kabir University of Technology, Tehran, Iran, 2003-2008

Research Interest

- Modeling of chemical contaminants adsorption and removal
- Design and implementation of experiments for nutrients removal from wastewater using adsorptive materials.
- Molecular dynamic simulation of the removal of contaminants of emerging concerns (CEC) using different filter materials.

Professional Experience

Assistant Professor, Faculty of Engineering, Golestan University, Golestan, Iran, 2021-present
Research Associate, Hydroinformatic Research group, Environmental Hazard Research Institute, Golestan University, Golestan, Iran, 2023-present
R&D Manager, Maah Banooye Zibaye Pars Inc., 2019-2021
Lecturer, Golestan University, Golestan, Iran, 2013-2021

- Basic principles and calculations in chemical engineering
- Water and wastewater treatment
- Fluid mechanics
- Adsorption phenomena

Skills

Programming (Matlab, C++, Python), Optimization, Molecular dynamics. Modeling and Simulation, Design Experiment.

Awards

- Top technologist of Golestan Province (2023)
- Top researcher of Golestan University (2023)

Current Projects

- Molecular dynamic simulation of removal of pollutants from water
- Molecular simulation of the removal of contaminants of emerging concerns (CEC) using different filter materials.
- Molecular simulation of carbon dioxide adsorption on porous adsorptive structures such as activated carbon, MXene, and metal-organic frameworks (MOF)

Publications

(* corresponding author)

F Badavar, **L. Lotfikatooli,** N. Hajilary. Enhancing Antifouling and Antibacterial Performance in Water Treatment: Development and MD Simulation of PES/PVA Composite Reinforced with MXene and ZnO. Water resources and industry. Submitted (under review).

M. R. Haghbin, M NiknamShahrak, **L. Lotfikatooli***, S. Mirzaei. Potential of Green-Based Microporous Carbon for Advanced Water Decontamination from Azo Dyes: Experiment and Molecular Dynamic Simulation Studies. Journal of Environmental Chemical Engineering. 2024.

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S. Mirzaei, **L. LotfiKatooli**, A. Ahmadpour, M. R. Haghbin, M NiknamShahrak, A. Arami-Niya. Potential of MOF-decorated porous carbons as a new-faced adsorbent for energy carrier gases storage: Experimental and simulation study. Chemical Engineering Research and Design, 2024.

S. Mirzaei, A. Ahmadpour, A. Shahsavand, A. Nakhaei Pour, **L. LotfiKatooli**, A. Garmroodi Asil, B. Pouladie, A. Arami-Niya. Experimental and simulation study of the effect of surface functional groups decoration on CH_4 and H_2 storage capacity of microporous carbons. Applied Surface Science, 2020.

L. Lotfikatooli, A. Shahsavand. An Innovative Approach for Molecular Simulation of Nano-Structured Adsorption Isotherms via Ant Colony Method. Physical Chemistry C, 2018.

L. Lotfikatooli, A. Shahsavand. Reliable prediction of adsorption isotherms via genetic algorithm molecular simulation, Journal of molecular modeling, 2017.

L. Lotfikatooli, A. Shahsavand. A Reliable Approach for Terminating the Genetic Algorithm Optimization Method. Iranian journal of numerical analysis and optimization, 2017.

L. Lotfikatooli, M.T Sadeghi. Hydrate: a promising platform for CO_2 Capture, Chemistry and Chemical engineering, 2011.

Presentations

L. LotfiKatooli. An Optimized Sampling Approach for Intelligent Searching Molecular Simulation Space, Division of Computers in Chemistry, ACS Spring 2020 National Meeting & Exposition.

L. Lotfikatooli, A. Shahsavand, F. Nazari. A Novel Method For Recruiting Global Optimization Techniques For Strategically Oriented Molecular Simulation. 11th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC). Munich, Germany, August 27 to September 1, 2017.

L. Lotfikatooli, M.T. Sadeghi, Prediction of Formation Conditions of Hydrogen + Tetrahydrofouran + Water System Using Artifitial Neural Network. 7th International Conference on Gas Hydrates (ICGH7). Edinburgh, Scotland, United Kingdom, July 17-21, 2011.

L. Lotfikatooli, K. Momeni, M.T. Sadeghi, Formation of CO_2 and $CH_4 + CO_2$ Hydrates Phase in Deep Ocean Porous Medium. Environmental Science and Technology Conference (ESTEC2009). Kuala Terengganu Malaysia, December 7-8, 2009.

Patent

- Peracetic Acid & Hydrogen Peroxide Measurement Kit, Iranian Research Organization for Science and Technology (IROST)

Synergistic Activity

- Director of Fanavar LILY Pars Company, Science and Technology Park of Golestan Province.
- Member of Golestan Province Engineering Organization.