Nasim Anousheh, PhD

RESEARCH SCIENTIST

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Profile

I am a Research Scientist at Indiana University, Department of Intelligent Systems Engineering (ISE). My research interests lie at the intersection of computational chemistry, machine learning and scientific visualization. I have a strong background in computational chemistry simulating different nanostructures, such as polymers, graphene, fullerenes, and carbon nanotubes. I also develop software to visualize these structures as they evolve in time. In addition, I'm a visiting lecturer for the Data Science Program at Indiana University. I teach data science courses focused on principles of data analysis, machine learning and implementations of these algorithms in different programming languages (Python, R and Spark).

Employment History

Visiting Lecturer for Data Science Program, Indiana University, Bloomington, IN, USA

May 2021 — Present

Research Scientist, Department of Intelligent Systems Engineering, Indiana University, Bloomington, IN, USA

September 2020 — Present

Postdoc, Department of Intelligent Systems Engineering, Indiana University, Bloomington, IN, USA

September 2018 — September 2020

Analytical Chemist, Rosoob-ab Ab Company, Tehran, Iran

September 2006 — September 2009

Responsibilities: Carrying out water quality tests such as pH; Turbidity; Total Dissolved Solids (TDS); Total Suspended Solid (TSS); Dissolved Oxygen (DO); Chemical Oxygen Demand (COD) and Total Organic Carbon (TOC). Analyzing the samples using Fourier Transform Infrared (FTIR) Spectroscopy.

Education

PhD in Physical Chemistry, University of Sherbrooke, Sherbrooke, QC, Canada

January 2011 — May 2017

My PhD research involves computational modeling and simulation of the polymers to design new materials with improved properties.

Title: *Atomistic Simulation of Fluoropolymers: Impact of Regiodefects on Characterization of Polyvinylidene Fluoride (PVDF)*

MSc in Physical Chemistry, Alzahra University, Tehran, Iran

September 2006 — December 2009

Title: Encapsulation of Hydrogen Molecule in Fullerene (C60)

Details

Nationality

Iranian, Canadian, USA

Green Card Holder

Links

https://www.anousheh.net

https://github.com/nasimanousheh

https://furiousatoms.com

Coding & Skills

Python

C++

R

Spark

LAMMPS

GROMACS

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BSc in Chemistry, Islamic Azad University, Tehran, Iran

September 2002 — June 2006

Journal Publications

1. **Anousheh, Nasim**, Azar Shamloo, Seifollah Jalili, and Jack A. Tuszynski. "Electrolyte adsorption in graphene and hexagonal boron nitride nanochannels." Journal of Molecular Liquids (2022): 120474.

2. J. C. S., Kadupitiya, **Nasim Anousheh**, Vikram Jadhao, Designing Machine Learning Surrogates using Outputs of Molecular Dynamics Simulations as Soft Labels". *arxiv.org/abs/2110.14714v1 (2021).*

3. Garyfallidis, Eleftherios, Serge Koudoro, Javier Guaje, Marc-Alex Côté, Soham Biswas, David Reagan, **Nasim Anousheh**, Filipi Silva, Geoffrey Fox, and Fury Contributors. "FURY: advanced scientific visualization." *Journal of Open Source Software* 6, no. 64 (2021): 3384.

4. Garyfallidis, Eleftherios, Shreyas Fadnavis, Jong Sung Park, Bramsh Qamar Chandio, Javier Guaje, Serge Koudoro, and **Nasim Anousheh**. "ThetA--fast and robust clustering via a distance parameter." *arXiv preprint arXiv:2102.07028* (2021).

5. Gau, Rémi, Stephanie Noble, Katja Heuer, Katherine L. Bottenhorn, Isil P. Bilgin, Yu-Fang Yang, Julia M. Huntenburg et al. "Brainhack: Developing a culture of open, inclusive, community-driven neuroscience." *Neuron* 109, no. 11 (2021): 1769-1775.

6. **Anousheh, Nasim**, Francisco J. Solis, and Vikram Jadhao. "Ionic structure and decay length in highly concentrated confined electrolytes." *AIP Advances* 10, no. 12 (2020): 125312.

7. **Anousheh, Nasim**, and Armand Soldera. "Influence of regio-irregular structures on thermal behaviour of PVDF." *Polymer* 125 (2017): 154-160.

8. **Anousheh, Nasim**, François Godey, and Armand Soldera. "Unveiling the impact of regioisomerism defects in the glass transition temperature of PVDF by the mean of the activation energy." *Journal of Polymer Science Part A: Polymer Chemistry* 55, no. 3 (2017): 419-426.

9. Okati, Afsaneh, Alireza Zolfaghari, Fariba Sadat Hashemi, **Nasim Anousheh-**, and HosseinZolfaghari Jooya. "Hydrogen Physisorption on Stone-Wales Defect-embedded Single-walled Carbon Nanotubes." *Fullerenes, Nanotubes and Carbon Nanostructures* 17, no. 3 (2009): 324-335.

Software

- **FURY - 3D Scientific Visualization**

I am a FURY core developer. FURY is a large community-supported open source software project for advanced scientific visualization. Visit https://fury.gl

Paper available here: Garyfallidis, Eleftherios, Serge Koudoro, Javier Guaje, Marc-Alex Côté, Soham Biswas, David Reagan, **Nasim Anousheh**, Filipi Silva, Geoffrey Fox, and Fury Contributors. "FURY: advanced scientific visualization." *Journal of Open Source Software* 6, no. 64 (2021): 3384.

- **nanoHUB - Ions in Nanoconfinement**

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I am co-creator of a web application for the simulation of Ions in Nanoconfinement, which is availble on nanoHUB. Visit nanoHUB.org

The app is available here: https://nanohub.org/resources/nanoconfinement

- **Furious Atoms (FA) Software**

I am the creator of Furious Atoms (FA). FA is an open source software for building, modifying and visualizing dynamic 3D chemical structures. Visit https://furiousatoms.com

Book Chapter

Handbook of Fluoropolymer

I wrote a chapter on Molecular Simulation of Fluoropolymer (chapter 6) for the Handbook of Fluoropolymer Science and Technology. This handbook is a comprehensive handbook on fluoropolymer synthesis, characterization, and processing.

The book is avalable here: Smith, Dennis W., Scott T. Iacono, and Suresh S. Iyer, eds. Handbook of fluoropolymer science and technology. John Wiley & Sons, 2014.

Teaching Experience

- **DSCI D590 - Data Science On-Ramp (May 2021- Present)**

This course is offered by Data Science Program, Indiana University and it contains many mini online courses. Each mini course is equal to one (1) credit hour. The courses are:

1. Data Processing, 2. Data Visualization Using Tableau, 3. Machine Learning with Python, 4. Machine Learning with R, 5. NLP in Python, 6. Web Scraping, 7. Basics of Scala, 8. Deep Learning Principles, 9. Introduction to Spark, 10. Kaggle Cases, 11. Machine Learning with Spark.

- **DS590 Data Science in Practice (Spring 2022- Present)**

DSIP is a graduate course offered in Spring and Fall semesters by Data Science Program, Indiana University. It is designed to help students gain critical, practical skills in applying data science to real world problems.

Mentoring Experience

Google Summer of Code

May 2021 — August 2021

I mentored the GSoC student to implement Molecular Surface and Ribbon Representations for Proteins with FURY. FURY is an open-source scientific visualization library in Python. The focus of the project is to provide a simple API and framework for large scale scientific animations.

More information about the project is available here:
https://blogs.python-gsoc.org/en/suntzunamis-blog/google-summer-of-code-final-work-product-1/

Results are available here:
https://fury.gl/latest/posts/2021/2021-06-08-week-1-sajag.html

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Recent Conferences

1. **Nasim Anousheh**, Javier Guaje, Filipi Silva, Serge Koudoro, Eleftherios Garyfallidis, Furious Atoms (FA) : open source software for building, modifying and visualizing dynamic 3D chemical structures, American Chemical Society Spring 2022.

2. **Anousheh, Nasim**, Francisco J. Solis, and Vikram Jadhao, Ionic Structure in Highly Concentrated Confined Electrolytes. American Physical Society March Meeting 2022.

3. J. C. S., Kadupitiya, **Nasim Anousheh**, Vikram Jadhao, Designing machine learning surrogate**s** using outputs of molecular dynamics simulations as soft labels. American Physical Society March Meeting **2022**.

Personal Characteristics

Driven, hard working, excellent team member, passionate.