Nasim Anousheh, PhD

LECTURER

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Profile

I am a Lecturer at Indiana University's Department of Intelligent Systems Engineering (ISE). My research interests are at the intersection of computational chemistry, machine learning, and scientific visualization. I teach data science courses that focus on principles of data analysis, machine learning, and the implementation of these algorithms in various programming languages, including Python, R, and PySpark.

Employment History

Lecturer, Department of Intelligent Systems Engineering, Indiana University, Bloomington

August 2023 — Present

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

May 2021 — July 2023

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

September 2020 — July 2023

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

September 2018 — September 2020

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)

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.

Links

https://www.anousheh.net

https://github.com/nasimanousheh

https://furiousatoms.com

Coding & Skills

Python

C++

R

PySpark

SQL

LAMMPS

GROMACS

"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**

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-D 590: Data Science On-Ramp
May 2021 — Present

This course is offered by the Data Science Program and consists of multiple mini online courses, each equivalent to one (1) credit hour. The courses include: 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 PySpark.

ISE-E 534: Big Data Applications

August 2023 — Present

This course is designed to provide graduate students with a comprehensive understanding of big data concepts, technologies, and their applications in the digital age. The course covers a range of topics, including IT fundamentals, cloud computing, PySpark, SQL, Hadoop and MapReduce, and AWS machine learning services.

ISE-E 221: Intelligent Systems I

August 2023 — Present

This course is designed to provide undergraduate students hands-on training in building intelligent systems using machine learning techniques. Through a combination of theoretical knowledge and practical application, students will gain a solid foundation in developing intelligent agents capable of decision-making, prediction, and learning. The course will focus on applying Scikit-Learn and TensorFlow to build and analyze intelligent systems.

DSCI-D 321: Data Representation

January 2024 — Present

This course is designed for undergraduate students to explore a wide range of data representations and processes integral to the data/information ecosystem. Emphasizing fundamental aspects and mechanisms of data engineering, the curriculum aims to equip students with the skills needed to prepare data effectively for applications and problem-solving in data science and machine learning.

ISE-E 332: Introduction to Modeling and Simulation

January 2024 — Present

The course is designed to provide an introduction to computational modeling and simulation techniques applied to nanoengineering. Undergraduate students will learn the basics of modeling, simulations, and parallel computing with a focus on applications in nanoengineering.

DSCI-D 592: Data Science in Practice

January 2022 — December 2022

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

Designing **machine learning surrogates** using outputs of molecular dynamics simulations as soft labels

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.