Workshop on

Artificial Intelligence and Machine Learning for Materials Science

11th to 15th December, 2023 (online mode)

Overview

The recent surge in high-performance computing, along with advances in big-data analytics, machine-learning (ML) and artificial intelligence (AI) methods has revolutionized various sectors of life, including business, health-care, and social media. Such techniques are also gaining tremendous attention in the broad engineering, materials science and chemistry community, especially due to their potential to advance fields of materials by design, accelerated synthesis, and materials characterization. To realize the full potential of machine learning and artificial intelligence for materials science applications, it is essential to combine them with *ab initio* methods, multiscale materials modeling, and experiments; this symposium aims to facilitate and strengthen such synergy.

This course, *to be held in the online mode* will focus on latest developments in artificial intelligence based techniques to (a) accelerate discovery of materials, (b) improve/accelerate synthesis protocols, (c) enhance existing characterization methods, and (d) develop robust, efficient, and accurate materials models, as well as simulation methods at multiple length scales; advances in ML/AI algorithms targeted towards materials chemistry applications will also be discussed. Broadly, this hands-on workshop will introduce students/postdocs, and industry scientists to recent successes of ML/AI in computational chemistry, materials synthesis/design/characterization as well as foster creative solutions to current challenges, and forge new frontiers in materials technologies *via* machine learning methods.

Objectives	▪ Exposing participants to the fundamentals of artificial intelligence (AI) and machine learning (ML) in the context of materials science and chemistry; ▪ Building in confidence and capability in the application of AI/ML tools and techniques and exposure to broad engineering/science topics where AI/ML tools/algorithms are currently employed; ▪ Providing exposure to practical problems and their solutions, through case studies and live projects in AI/ML applied to materials/chemistry; ▪ Enhancing the capability of the participants to solve problems in engineering system by leveraging AI/ML tools and algorithms.

Modules	▪ Overview of Materials design and discovery, computational structure-property relationships in materials ▪ Brief introduction to data science, data visualization and analysis ▪ Overview of AI/ML techniques ▪ Datasets and Databases ▪ Multi-fidelity scale bridging using AI/ML with an emphasis on molecular simulations. ▪ Inverse design using AI/ML – from evolutionary algorithms to deep learning ▪ AI/ML techniques for: - Materials characterization - Autonomous experiments - Computer vision and image classification - Force-field parametrization - Structure optimization ▪ Hands-on problem-solving pertaining to all the modules above.
You should attend if…	▪ You are student (BTech/MTech/PhD) or faculty member from Materials Science/Chemical/Chemistry/Mechanical or allied departments. ▪ You are executive, engineer or researcher from manufacturing, service and government organizations including R&D laboratories.
Registration	One-time GIAN Registration: Please visit http://www.gian.iitkgp.ac.in/GREGN/index and register by paying a one-time registration fee of Rs 500/- (those who have already registered on the GIAN portal need not pay again.) Select the current course under the course registration tab and save. After this step, please email the course coordinator with proof of your course registration along with your basic details. You will be informed if you are selected, and you can pay the required participation fee for the course as follows: The participation fee for the course is as follows (inclusive of 18% GST): **Participants from abroad:** USD 250 **Industry:** INR 8,000 **Faculty/staff from Academic/Research institutions:** INR 4000 **Students:** INR 2000 A certificate of completion will be issued upon satisfactory attendance. For any questions regarding registration or other practical information, please contact the course coordinator. Information about the course will be posted on https://events.iitgn.ac.in/2023/ai-ml-materials/ **Dates:** December 11-15, 2023 **Timings:** 10 AM to 4 PM (tentative) **Online meeting link will be shared with the selected participants**

The Faculty

Subramanian Sankaranarayanan is an Associate Professor in the Mechanical Engineering department at University of Illinois Chicago and the Group Leader of the theory and modeling group in the Nanoscale Science and Technology Division at Argonne National Laboratory. He is also a Senior Fellow at the Institute of Molecular Engineering at University of Chicago. Prior to joining Argonne, Subramanian was a post-doctoral fellow at the School of Engineering and Applied Sciences at Harvard University. His research focuses on the use of machine learning to bridge the electronic, atomistic and mesoscopic scales for accelerated materials discovery and design. Other programmatic efforts include development and use of AI algorithms for inverse design of materials and deep learning for integrated X-ray imaging of ultrafast energy transport across solid-solid and solid-liquid interfaces. His interests span a diverse range of applications from energy storage, tribology, corrosion to neuromorphic computing and thermal management.

Host Faculty

Raghavan Ranganathan is an Assistant Professor in the discipline of Materials Science and Engineering at Indian Institute of Technology, Gandhinagar, India. He received his B. Tech in Metallurgical and Materials Engineering from IIT Madras and Ph.D. in Materials Science and Engineering from Rensselaer Polytechnic Institute in 2016. His research focuses on atomistic and molecular simulations coupled with AI and ML applications to uncover structure-property relations in materials, with a focus on properties such as mechanical, thermal, mass transport and reactive processes in a host of materials.

Course Coordinator

Dr. Raghavan Ranganathan
Phone: 079 2395 2557
E-mail: rraghav@iitgn.ac.in

GIAN Portal registration:
http://www.gian.iitkgp.ac.in/GREGN/index

Course website:
https://events.iitgn.ac.in/2023/ai-ml-materials/