

# Artificial Intelligence and Machine Learning for Materials Science

## 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 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.

<b>Objectives</b>	<ul style="list-style-type: none"><li>▪ Exposing participants to the fundamentals of artificial intelligence (AI) and machine learning (ML) in the context of materials science and chemistry;</li><li>▪ 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;</li><li>▪ Providing exposure to practical problems and their solutions, through case studies and live projects in AI/ML applied to materials/chemistry;</li><li>▪ Enhancing the capability of the participants to solve problems in engineering system by leveraging AI/ML tools and algorithms.</li></ul>
<b>Modules</b>	<ul style="list-style-type: none"><li>▪ Materials design and discovery, computational structure-property relationships in materials</li><li>▪ Overview of AI/ML techniques</li><li>▪ Multi-fidelity scale bridging using AI/ML with an emphasis on molecular simulations.</li><li>▪ Inverse design using AI/ML – from evolutionary algorithms to deep learning</li><li>▪ AI/ML for materials characterization</li><li>▪ AI/ML for autonomous experiments</li><li>▪ Hands-on problem-solving pertaining to all the modules above.</li></ul>

<b>You should attend if...</b>	<ul style="list-style-type: none"> <li>▪ You are student (BTech/MTech/PhD) or faculty member from Materials Science/Chemical/Chemistry/Mechanical or allied departments.</li> <li>▪ You are executive, engineer or researcher from manufacturing, service and government organizations including R&amp;D laboratories.</li> </ul>
<b>Registration</b>	<p>The participation fee for the course is as follows (18% GST will be applicable as per norms):</p> <p><b>Participants from abroad:</b> USD 250  <b>From SAARC:</b> USD 150  <b>Industry:</b> Rs. 12,000  <b>Research Organizations:</b> Rs. 8000  <b>Faculty/staff from Academic institutions:</b> Rs. 5000  <b>Students:</b> Rs. 1500</p> <p>The above fees include all instructional materials, computer use for tutorials and internet facility at the host institute during the course. The participants must take care of their travel. Accommodation can be arranged for participants on first-come-first-served basis for nominal payment. For any questions regarding registration or other practical information, please contact the course coordinator.</p> <p>Information about the course will be posted on <a href="http://events.iitgn.ac.in/2020/ai-ml-materials/">http://events.iitgn.ac.in/2020/ai-ml-materials/</a></p> <p><b>Dates:</b> July 20 – 24, 2020 (Subject to change due to COVID-19 pandemic)  <b>Venue:</b> IIT Gandhinagar</p>

## 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/molecular simulations 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 Co-ordinator

**Prof. Raghavan Ranganathan**

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GIAN Portal registration:

<http://www.gian.iitkgp.ac.in/GREGN>

Course website:

<http://events.iitgn.ac.in/2020/ai-ml-materials/>