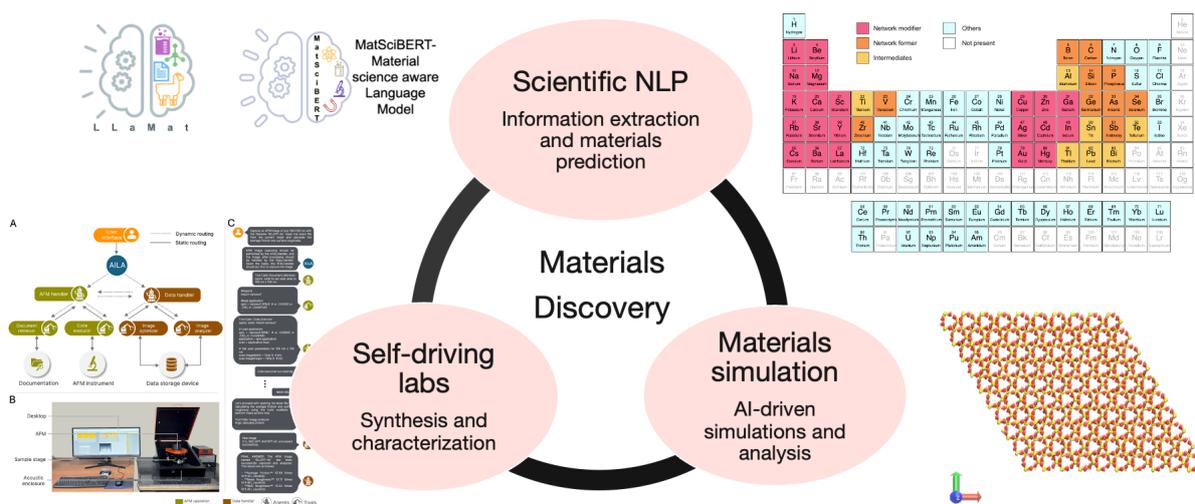


Artificial Intelligence for End-to-End Materials Modeling and Discovery

The development of artificial intelligence (AI) systems for scientific discovery presents unique challenges that differ significantly from traditional AI applications. In this talk, we will discuss an end-to-end AI framework that addresses these challenges, using materials discovery as a compelling use case. We will explore how AI approaches can transform a traditionally sequential and time-intensive process into an efficient computational workflow. The discussion will center on a three-tier AI system architecture: (i) specialized large language models (LLMs) and other information extraction models incorporating domain-specific knowledge representations for intelligent search space reduction, (ii) graph neural networks that combine physics-based inductive biases for materials simulation, and (iii) LLM agents for automated experiments. Through practical demonstrations, we will examine how these AI components handle complex scientific problems, particularly focusing on information extraction from tables, generative modeling of crystal structures, and atomistic modeling of materials. We will analyze the integration of physical constraints and domain knowledge into neural architectures, demonstrating how this enhances model interpretability and generalization. The talk concludes by examining open problems in scientific AI, including causal discovery, out-of-distribution generalization, and the seamless integration of symbolic and neural reasoning for scientific applications.





Prof. N. M. Anoop Krishnan, IIT Delhi

Biosketch

Prof. N. M. Anoop Krishnan is an Associate Professor in the Department of Civil Engineering, IIT Delhi with a joint appointment in the Yardi School of Artificial Intelligence. Anoop completed his Ph.D. in Civil Engineering from Indian Institute of Science Bangalore in 2015, after which, he worked as a postdoctoral researcher in University of California Los Angeles from 2015 to 2017. Prior to this, he completed his B.Tech. in Civil Engineering from National Institute of Technology Calicut in 2009. He works at the intersection of materials, mechanics, simulations, and AI and ML with the goal of accelerating materials modeling and discovery. He has published more than 120 international peer-reviewed journal publications and has 2 granted patents. He has won several awards including Sir A. Pilkington Award by Society of Glass Technology, UK (2024), Alexander von Humboldt Fellowship (2023) for experienced researchers, Google Research Scholar Award (2023), W. A. Weyl International Glass Science Award by International Commission on Glass (2022), Indian National Academy of Engineering Young Engineer Award (INAE YAE 2020), BRNS-DAE Young Scientist Award (2021), Indian Academy of Sciences Associateship (2022), and National Academy of Science India Young Scientist Award (NASI YSA 2021).