ME Seminar

Towards Explainable & Interpretable AI for Materials Design

Prof. Sid Kumar, TU Delft, Netherlands

ABSTRACT

Designing materials to meet specific physical property requirements is a time-intensive process, often marked by resource-heavy experiments and the occasional “Eureka!” moment. Machine learning (ML) offers potential to streamline the design process, but barriers like data scarcity and the black-box nature of many models hinder the practical transition from computational predictions to lab synthesis or manufacturing. Drawing on findings from our recent studies, this talk will explore how incorporating explainability and interpretability into ML models can leverage prior physics and mechanics knowledge to accelerate the discovery of new materials. Specifically, I will present how attention-based deep learning models can facilitate the explainability of structure-property relations in nanoporous polymers, such as covalent organic frameworks. Likewise, I will demonstrate how interpretable latent space-based deep learning models can enable automated, yet human-in-the-loop, design of self-healing vitrimeric polymers with desired properties. Beyond polymers, I will briefly highlight similar applications of explainable and interpretable ML for designing metamaterials with tailored mechanical properties. These advancements illustrate how explainable and interpretable ML can accelerate the discovery of novel, sustainable (meta-)materials with desirable properties.

ABOUT THE SPEAKER

Dr. Sid Kumar is an Assistant Professor at TU Delft in the Department of Material Science and Engineering and Faculty of Mechanical Engineering since 2021, where he leads the Mechanics, Materials, and Computing group. He obtained his Ph.D. in Aeronautics from Caltech followed by a postdoc position at ETH Zürich. Previously, he obtained a dual M.S. from Caltech and Ecole Polytechnique (France). Sid has been awarded the Dutch Research Council (NWO) Veni award, the Foster and Coco Stanback fellowship in Engineering and Applied Science at Caltech, and the University of Paris Saclay fellowship at Ecole Polytechnique. His research interests lie at the intersection of mechanics of materials, computational modeling, and machine learning — with a focus on inverse problems in materials design and modeling.

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