Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad – 500 046

Webinar

Autonomous Computational Discovery of Sustainable Energy Materials

Koushik Pal

Northwestern University, IL

The discovery of new materials is an important yet challenging task as trial-and-error methods of synthesising novel compounds in the laboratory can be extremely labour, time, and cost-intensive. Computational methods have the potential to reduce all three factors. In this talk, I will focus on the autonomous discovery of a class of energy materials having low lattice thermal conductivities and promising thermoelectric performance using advanced computational methodologies. First, I will show how the rational design of an autonomous workflow can accelerate the discovery of thermodynamically stable compounds based on high-throughput density functional theory calculations. Then, I will demonstrate how a machine-learning model based on the crystal graph convolutional neural network can help to discover the 'hidden' compounds in the same family of materials that would otherwise be difficult to do in conventional ways. Finally, I will show how data-driven discovery unravels novel physical insights behind the unusual thermal transport in some predicted compounds, providing new avenues for research and exploration.

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4:00 PM