



Diving Deep Into Physics
A Seminar Series of The
Department of Physics

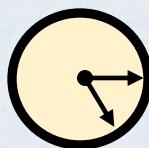
IIT
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Seminar on
From Empirical to Machine Learning Potentials: Modeling
Liquid Ethylene Glycol
By
Dr. Anjali Gaur
Jawaharlal Nehru Centre For Advanced Scientific Research,
Bengaluru



Jan 6, 2025



05:00 PM to 06:00 PM

About the Speaker

Dr. Anjali Gaur completed her Ph.D. under the guidance of Prof. Balasubramanian Sundaram at JNCASR, Bengaluru. Her doctoral research focused on force field development for liquids and investigating their physical properties using ab initio and classical molecular dynamics simulations. Currently, she is working on the development of machine learning potentials for liquid ethylene glycol. As a postdoctoral researcher, she will join the PHENIX CNRS lab to work with Prof. Mathieu Salanne on the development of machine learning-based classical force fields for battery electrolytes.

Venue: Kothari Seminar Hall, Department of Physics