UNIVERSITÄT BAYREUTH

OPTEXC

invited speaker series

Chemistry, Complexity, and Computation: Modelling Reactivity in Energy Materials*

Materials such as 2D materials, MOFs, high-entropy alloys, carbon nanotubes, and perovskites are driving innovations in energy storage and conversion. Understanding their synthesis and behavior under physicochemical constraints requires establishing structure-property relationships across multiple length and time scales. In this talk, I will discuss how large-scale reactive molecular dynamics with quantum mechanical simulations can bridge these scales. The talk will also introduce the fundamentals of ReaxFF, including eReaxFF, a recent extension that enables the explicit modeling of electron dynamics in reactive systems.

Date: Tuesday, 11th Nov 2025

Time: 12.30 pm

Room: S 621 (NW II)

Dr. Swarit Dwivedi
Monash University
Australia