Atomic Choreography: Coupled Dynamics of Molecular Machines in Metal-Organic Frameworks

Saeed Amirjalayer

Interdisciplinary Center for Scientific Computing, Heidelberg University

Responsive materials o/en exhibit complex and nonlinear behavior when subjected to external stimuli. A particularly promising approach to harnessing and controlling such responses is the integration of molecular machines and switches within tunable host environments, such as metal–organic frameworks. This strategy enables precise control over motion, switching, and adaptive responses at the molecular level. Beyond fundamental interest, a detailed understanding of the dynamic processes governing these responses is essential for the rational design of functional materials. In this presentation, I will provide an overview of our work on developing and applying theoretical methods in atomistic investigations of molecular switches and molecular machines within functional materials, including metal–organic frameworks. I will emphasize how intermolecular interactions, framework topology, and confinement influence dynamics at the molecular level, making it possible to systematically tailor the functionality of these responsive materials.