

iCeMS Kitagawa Group Seminar



Prof. Saeed Amirjalayer

Interdisciplinary Center for
Scientific Computing
University of Heidelberg

“Elucidating Dynamic Phenomena in Responsive and Functional Materials”

[You can find more information here \(click or scan\)](#)

Date: May 22nd, 2025
Time: 13:00-14:00
Place: 2F Seminar room,
iCeMS main bldg.



Abstract: This presentation highlights the use of atomistic simulations to investigate dynamic behaviors in responsive materials such as functionalized surfaces, molecular crystals, and porous frameworks. By examining how intermolecular interactions and confinement influence individual and collective dynamics, and integrating simulations with advanced experiments, the work offers mechanistic insights that guide the design of next-generation materials for applications in catalysis, actuation, and energy conversion.

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