UNIVERSITÄT DUISBURG ESSEN

Offen im Denken

Theorie-Kolloquium WS 2025/26
Fr 12.12.2025, 14:00-15:30
MC 351 & online (URL in E-Mail)

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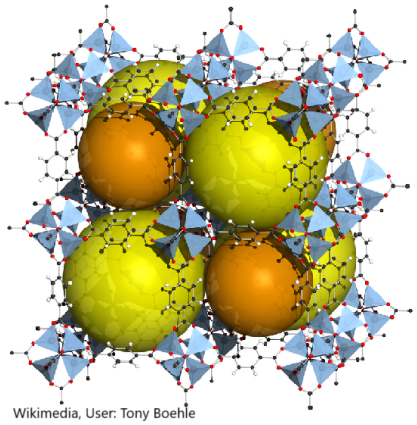
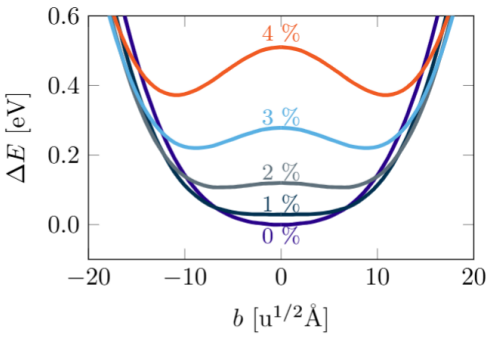
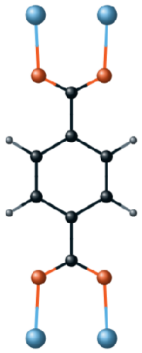
Collective Buckling in Metal-Organic Framework Materials

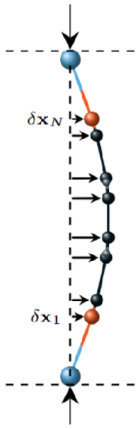
Dr. Nico Hahn

Chalmers University of Technology









Metal-organic frameworks (MOFs) are crystalline materials consisting of metallic coordination centers connected by organic linkers, forming highly porous and flexible structures. In this talk, I present a theoretical framework that captures how these linkers can undergo collective buckling under compressive strain. Starting from the atomic structure of a single linker, we define a buckling coordinate whose effective potential takes the form of a double well. Interactions between linkers arise from dipole-dipole coupling, leading to a lattice Hamiltonian that exhibits a transition between an ordered ferrobuckling phase and a disordered phase.

As an application of the theory, we consider the prototypical framework MOF-5. Using density functional theory, we obtain the model parameters and show that collective buckling can occur under moderate uniaxial strain and experimentally accessible temperatures.

Finally, we discuss the low-temperature regime where quantum effects can become relevant and show that our model reduces to a transverse-field Ising model, allowing for a parabuckling state.

N. Hahn, L. Öhrström, R. M. Geilhufe, arXiv:2511.16286