Investigating cooperative and correlated multiscale phenomena in reticular materials through the micromechanical model: MicMec

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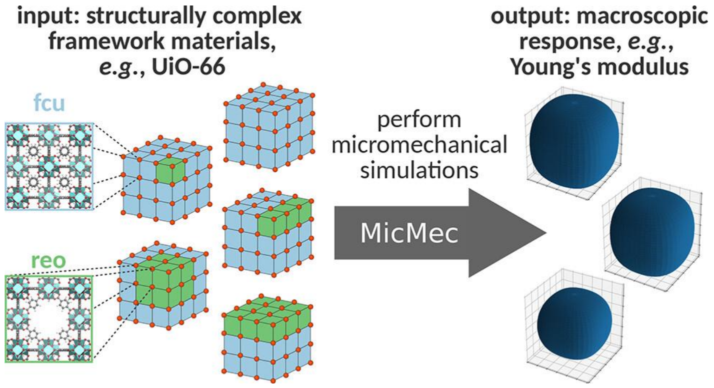
Disorder strongly impacts reticular materials, varying from ångström-sized atomic substitutions to micrometre-sized crystal interfaces.[1,2] Because different types of disorder interact, they cooperatively alter the macroscopic behaviour of these materials on even much longer length scales,[1] which calls for dedicated simulation techniques that bridge atomic information with macroscopic phenomena.

Herein, we explore how the micromechanical model,[2] as implemented in MicMec (github.com/molmod/micmec),[3] tackles this computational challenge. The micromechanical model is a coarse-grained technique consisting of two ingredients. It starts from the observation that reticular materials can be partitioned into nanometre-sized unit cells. First, it calls for mapping these atomic unit cells to the micromechanical interaction beads, which coincide with the corner positions of these cells. Second, it describes that these micromechanical beads interact with one another via an effective Hamiltonian governed by the elastic deformation energy, which is itself defined based on the atomically accessible stiffness tensor of the unit cell.[2] In contrast to earlier coarse-grained techniques for reticular materials,[4] the micromechanical model achieves a reduction in interaction beads of two to three orders of magnitude while preserving the material's topology, as topology is the most critical descriptor for a material's stability.[5] It considers any nonreactive polymorphism in the material and can be adopted to access longer length and time scales in a hierarchical approach.

This talk will highlight the rationale behind the micromechanical model and its implementation and demonstrate how it can be adopted to model the impact of correlated defects on the mechanical properties of the prototypical UiO-66 metal-organic framework as a case study.[1,3] We will also discuss the theoretically achievable speed-up using this method and the current limitations of the model. Finally, we will also briefly explore how the micromechanical model also forms the basis for strain engineering, *e.g.*, by constructing flexible crumple zones in the otherwise rigid UiO-66 material.[6]



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Acknowledgements. Funded by the European Union through ERC-StG-2023 STRAINSWITCH (grant no. 101115787). Views and opinions expressed are however those of the authors only and do not necessarily reflect those of the European Union or the European Research Council. Neither the European Union nor the granting authority can be held responsible for them.