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Multiscale diffusion in porous media: From interfacial dynamics to hierarchical porosity

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The transport of liquid and solutes in porous media over widely different time and length scales, ranging from specific interactions with the surface (and the associated interfacial dynamics) to the effective pore diffusion through hierarchical porosity, is central to many environmental and technological processes. This interplay between surface functionality and hierarchical porosity requires, on the one hand, a detailed molecular-level picture of sorption, reaction, and mobility, and realistic geometrical models of hierarchically porous media on the other, to establish (and apply) quantitative morphology–functionality–transport relationships for the tailored preparation of ever more selective and efficient materials for storage, separation, and catalysis.

We present a modelling approach that allows us to determine effective transport properties covering a hierarchy of length scales, from the detailed molecular-level picture at the surface and the interfacial dynamics, emerging from molecular dynamics (MD) simulations [1], to diffusion in physical reconstructions of hierarchical porosity, simulated by a Brownian dynamics approach [2,3].

A key message of this work is that interfacial phenomena resolved by the MD simulations have a strong influence on the effective diffusivity resulting on a macroscopic scale, an effect that is usually difficult to assess and quantify or even remains unknown. This influence can be adequately reflected by the presented multiscale simulation approach, which embeds the relevant interfacial dynamics along the hierarchical porosity and associated molecular diffusion path.

References

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