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Understanding Hindered Diffusion & Flow in Hierarchical Porous Networks Combining Electron Tomography and Pore-Scale Simulations

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Disordered hierarchical porous media play a crucial role as fixed bed supports for a wide range of applications from separation techniques such as HPLC to heterogeneous catalysis. To understand and ultimately optimize their performance, the relationship between morphology and transport properties has to be established. The key is a statistically meaningful, quantitative description of the pore structure as basis for pore-scale simulations to determine flow and diffusion properties using realistic models for the macro and mesopores (Figure 1) [1-3].

A combination of FIB slice&view and (S)TEM tomography is used to address the length scales and resolution needed to represent the macro- and the mesopore space. [4, 5] An accurate segmentation of the 3D reconstructions is one of the most critical steps to build meaningful models, both for a quantitative morphological description as well as for simulation of flow and diffusion properties. In addition to various image processing steps to reduce noise and artifacts as preprocessing for a segmentation, we have quantitatively analyzed SIRT and DART reconstructions of disordered mesoporous materials to evaluate the reliability of the reconstruction and how the reconstruction affects the morphological description and the diffusion properties. The flow and diffusion simulations are performed based on a subarea of the reconstruction with periodic mirror boundary conditions using the lattice-Boltzmann method and the random walk particle tracking respectively. [1-3] Furthermore, hindered diffusion, explicitly taking into account the solute vs. pore size ratio, is simulated to derive a quantitative expression of the hindrance factor, which describes the degree to which diffusion through a material is hindered compared to the diffusion in the bulk liquid depending on the size ratio.

The possibilities for understanding the role of the macro- and mesopore structure will be illustrated using application examples of silica monoliths and packed spheres in HPLC as well as disordered carbon supports used in catalysis together with a discussion of the reliability of the measurements and simulation. This ranges from a quantitative evaluation of the pore morphology depending on synthetic parameters and wall effects in HPLC packing to the development of a master curve describing hindered diffusion without specific surface interactions for all materials with comparable morphology, which potentially encompasses all sol-gel processed mesoporous silicas. Details on the image acquisition, reconstructed microstructure morphology and the simulations will be presented and the crucial role of combining experiment and modelling discussed [6].

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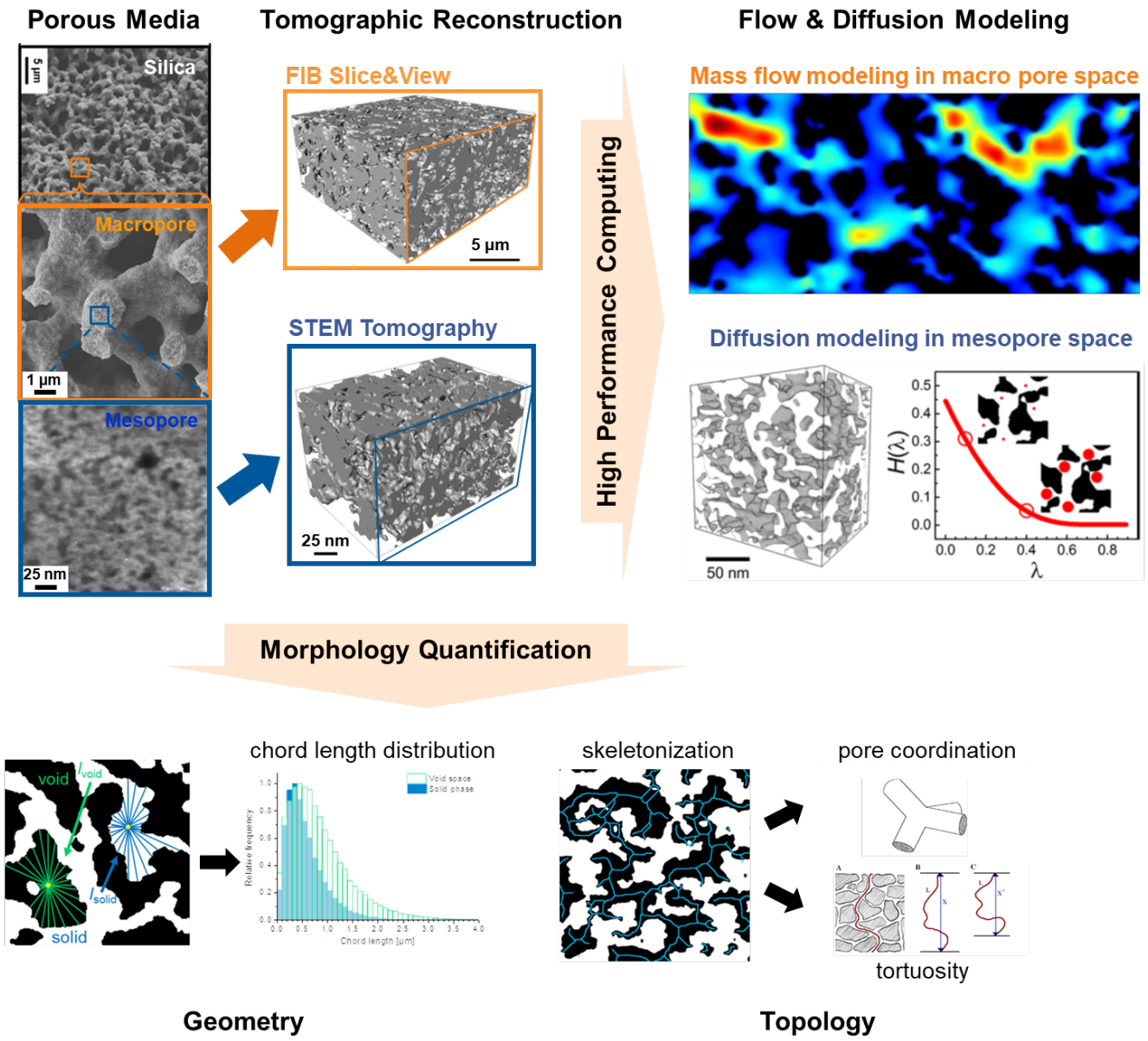

Figure 1. Understanding the role of the pore structure in hierarchical porous media: from tomographic reconstructions to a quantitative morphological description and flow & diffusion properties.

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