

## Computational design and optimization of porous heterogeneous hierarchical materials

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The application of porous heterogeneous hierarchical materials across industries is limitless; their roles as catalysts, adsorbents, ion-exchangers, membranes, antibacterial agents, etc., are constrained only by the ability to design and fabricate new materials systems optimized for various reactive transport processes. These materials often comprise an inert scaffold designed with multiple levels and distributions of porosities, tortuosities and particle sizes, which are decorated with active sites. While the hierarchical structure and chemical composition of such materials are inextricably linked, most design schemes focus on one aspect or another, owing to the complexity in such a holistic design. By coupling rigorous computational and experimental approaches we are developing a new design paradigm that considers both the material properties along with the fabrication and structural aspects of the material system. In this talk we will discuss initial results including the design and optimization of an activated carbon based flue gas filter.