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Modeling and Simulations of Nanoporous Materials: Design and Function

Guest Editor:

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Deadline for manuscript submissions:
closed (20 November 2023)

Message from the Guest Editor

Dear Colleagues,

Nanoporous materials are now widespread in the chemical industry and in biomedical devices. Rapid progress in computational power and modeling techniques has enabled the physics- and data-driven discovery of new material structures and the optimization of their functions. This Special Issue presents recent advances in the fundamentals, methodology and applications of molecular simulations for the computational design of nanoporous materials and their applications.

We welcome submissions on but not limited to:

- simulation design of microporous solids;
- amorphous carbons and silicas with tailored pore-size distributions;
- data-driven approaches to nanomaterials design;
- tailoring nanoporous materials to particular applications;
- exploration of chemical space in pursuit of new porous structures, such as new zeolites, MOFs, etc;
- traditional simulations of adsorption, separation and transport in nanopores.

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Message from the Editor-in-Chief

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