Pore Topology and Surface Design for Energy Storage Applications

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Thermal energy storage based on the adsorption of a working fluid (e.g. water) inside a microporous material offers the possibility to achieve high energy storage capacities. The optimization of the porous material is a high-dimensional problem that needs to consider not only the material properties and the working fluid, but also the thermodynamic process used for (dis)charging the fluid, resulting in a mixed integer non-linear optimization problem. We use classical molecular simulations for predicting adsorption properties of a working fluid with a microporous material e.g. zeolites or covalent / metal organic frameworks (COFs / MOFs) respectively. Classical density functional theory is applied as a surrogate model to allow for a full process optimization. The optimization of the energy storage process and of the microporous material is performed using the surrogate model with iterative refinement from molecular simulations. Based on a target function defined for the energy storage process, the proposed method comprises two steps. First, an optimal (hypothetical) potential energy surface is obtained, which represents the porous material. Second, a real material is selected that best resembles the optimal (hypothetical) potential energy surface.