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Strategies for Hydrogen Storage in Nanoporous Metal-Organic Framework Materials

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Storing hydrogen by physisorption in porous materials is a challenging problem of great interest for future vehicle technology. Metal-organic frameworks (MOFs) are a new class of nanoporous materials that have demonstrated exciting potential for solving this problem. MOFs are synthesized by the self-assembly of metal nodes and connecting organic linker molecules to create stable, porous frameworks. The synthetic chemistry opens the possibility to create an almost unlimited number of MOFs and to tailor them for particular applications, such as hydrogen storage. The diversity of MOFs also creates an opportunity to learn more about the fundamentals of hydrogen adsorption in porous materials. We have used a combination of classical Monte Carlo simulations and quantum mechanical approaches to investigate fundamental questions about hydrogen storage in MOFs and to design new materials with improved storage capabilities. Relationships have been elucidated between hydrogen uptake and properties such as the MOF surface area, void volume, degree of catenation, enthalpy of adsorption, and cation content. Introduction of cations is a promising strategy to improve hydrogen uptake at room temperature, and different metal cations and different strategies for introducing them into MOFs have been screened computationally.