

Computational Porous Materials Design and Applications

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In this work, I will present our group's recent effort in using the principles of rational materials design to facilitate synthesis of metal-organic framework (MOF) composite materials. In particular, we focus on designing MOF@MOF materials using the algorithm developed within our lab and our theoretical predictions have led to discovery/synthesis of new composite porous materials. Finally, we apply our computational tools to help facilitate synthesis of new chemiresistive sensor materials with excellent performance for toxic gas detection.