

USF NEXUS INITIATIVE 2019 AWARD RECIPIENT

Brian Space

An Iterative Design Process for Functional Porous Materials: Modeling Meets the Laboratory

Flexible porous materials with tunability can solve the methane (NG) storage and hydrocarbon separation problem. A decade of study of porous material design, along with modeling and analysis of molecular interactions can now be brought to bear on creating superior storage materials for NG in metal-organic framework materials, MOFs. Through iterative design between experiment and modeling, flexible materials that show a step wise expansion in response to methane can surmount extant technical challenges. Here, the object is to use previous insights developed through synthesis and quantitative modeling of rigid MOFs in an established synergistic theoretical / experimental team to create, modify and evaluate flexible MOFs for NG storage and release.

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