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First-principles study of van der Waals driven molecular sponges as carriers for small molecules MAJID MORTAZAVI, Fritz-Haber-Institut der Max-Planck-Gesellschaft, ALEXANDRE TKATCHENKO, Fritz-Haber-Institut der Max-Planck-Gesellschaft;Physics and Materials Science Research Unit, University of Luxembourg — Molecular sponges are crystal materials with molecular building blocks glued together by van der Waals (vdW) interactions acting as hosts to incorporate guests within their pores. A recent example is Tetrakis(dimethloxyphenyl)adamantane (TDA) with branched adamantane scaffolds demonstrating a remarkable ability to capture/release a wide range of small molecules [1]. While various TDA-based inclusion complexes have been synthesized, the underlying principles of formation of these complexes remain puzzling [1]. Using vdW-inclusive DFT calculations we study the formation of inclusion complexes with several small molecules via full structural relaxation and stability analysis, and subsequently proposing several possible formation mechanisms for the inclusion compounds. Based on formation energies we predict a selective molecular capture depending on the class of TDA hosts. The selective response is closely correlated to the structural features of TDA crystals, such as lattice energies and pore sizes. The insights gained in our work are beneficial for engineering TDA-based sponges for diverse practical applications including storage of hazardous and explosives materials, and potential uses in medicine and materials science. [1] Angew. Chem. 128/13910 (2016).

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