The effect of the MOF framework on electronic and structural properties of the encapsulated guest species

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Nanoporous materials can be classified based on their type as well as their functionality, which are determined by their intended practical applications [1]. The development of efficient nanoporous materials for various applications, such as gas adsorption and separation, drug delivery, molecular sensing, energy storage in batteries, and catalysis, hinges on a thorough understanding of the chemical and physical changes that occur in the target species upon adsorption. For example, in collaboration with experimentalists, the concept of using a designable regular MOF material could be applied to create a highly stable, selective adsorption system [2]. Recently, the adsorption and photo-polymerization of P_4 molecules encapsulated in an indium(III)-based metal-organic framework, resulting in a double-helical chain composite comprising [P_8] units, have been reported [3]. This provides direct crystallographic evidence for the structural building blocks of red phosphorus, stabilized within the pores of a metal-organic host. Our study confirmed that the optimal number of monomers and their configurations, due to guest-host and guest-guest interactions, are suitable for forming a thermodynamically stable double helix $[P_8]_n$ structure within the environment of the 3D channels. These data clearly demonstrate the applicability of the obtained material for visible light-induced water treatment and its potential for use in artificial photosynthesis processes.

References

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