Design of new porous supramolecular arrays from flavyliums derivative linker. A theoretical assemble toward surface properties

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Abstract

Here, we attempt to design novel microporous framework materials, in this sense, such designs were carried out taking flavylium derivatives as corresponding linkers, which are assembled with the chosen well-known secondary building units SBUs such as $Zn_4O(CO_2)_6$ and MIL-53 respectively. The linkers and SBUs are put together by means of topological simulations taking advantage of the powerful AutoGraFS tool, which allows a screening of feasible supramolecular frameworks, and therefore, these initial designs are validated from the molecular mechanics until highly accurate quantum mechanics techniques. Therefore, we selected the most stable structures through tight binding DFTB and DFT periodic computations, this finding enables us to obtain the lattice vectors and the unit cell parameter [a,b,c], achieving the simulation of their overall structural accurate description. Later the grand canonical Monte Carlo simulations (GCMC) give rise to the best elucidation of the active surface properties, including surface area, pore volume, and size, and several calculations to the host-guest gas adsorption characteristics and thus contrast the intrinsic capacities and applications of such novel designs. Additionally, these frameworks depict favorable candidates for a post-synthetic work that is bearing by a strategic cutting-edge research.

Author keywords

Adsorption Isotherm; Electronic structure; MOFs design