

Computational Screening of Hetero-type Core-Shell Metal Organic Frameworks

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Up to now, existing core-shell metal organic frameworks (MOFs) consisted of two MOFs which have exactly same topology. This restriction puts a ceiling on synthesizing diverse core-shell structures that can possess synergetic properties and serve dual functionalities. To go beyond this current limitation, we constructed an algorithm that can match different core and shell MOF materials. At first, we selected MOF-5 which is most simple structure as test case material and searched the existing MOF structures within the CSD MOF database to find a potential match. As a result, several structures were identified to be a match with the MOF-5 structure. By extension, we used our algorithm with cubic and hexagonal unit cells among CSD MOF database and the candidate pairs of core-shell structure were identified.