Construction of MOF Structures from Topology and Building Blocks

이상원, 김지한[1,†]

한국과학기술원; [1]한국과학기술원 생명화학공학과

(jihankim@kaist.ac.kr[†])

We have developed a python library for the construction of metal-organic framework (MOF) structures from the topology and the building blocks. The library includes a parser for the topology information file of "cgd" format from the RCSR database. The topology structures are relaxed according to the given building blocks. For the relaxation of the topology, we have implemented the objective function using the automatic differentiation of Tensorflow 2 to use the gradient information. The gradients obtained from the automatic differentiation significantly improve the speed of optimization of the topology. For that reason, this library can handle topologies of a large number of vertices and edges without limitations. The orientation and permutation searching algorithm developed in this work can locate a building block to the assigned node in any kind of topologies while the previous works on MOF construction only offer limited kind of topologies. From the results, this library generated almost infinite number of MOF structures from the finite number of building blocks and topologies. We expect that the result significantly influences screening works on MOFs and MOF applications.