Partial Amorphization of Metal-Organic Frameworks to Enhance Their Surface Area for Gas Adsorption

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Metal-organic frameworks (MOFs) are porous materials with extraordinary surface area, which make them appealing options for gas adsorption. Thus, many researches have focused on the perfect crystalline MOFs, while the amorphous phases received less attention. Since, amorphization of the majority of MOFs can drop their accessible porosity and negatively affect their gas adsorption capabilities. In present study, we reveal some exceptional cases wherein the partially-amorphized structures exhibits favorable enhancement in accessible surface area compared to the perfect crystalline counter-parts. These MOF contain non-accessible regions in the form of closed pockets. Here, we applied shear stress to rupture these non-accessible pockets, using reactive molecular dynamics simulation. The results show that more than 40% increase in accessible surface area can be reached after applying the shear stain. Present work, demonstrates that partial amorphization of some MOFs can beneficially create new surfaces for gas adsorption.