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Hydrogen adsorption of Ti decorations in Mg-Metal Organic Framework-74: A First-Principles Study

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Metal-Organic Frameworks show to be one of the most promising materials for hydrogen storage materials owing to containing lots of hydrogen trapping sites, tunable pore size and cheap to produce. However, the hydrogen adsorption energy of these materials is very low. In the present work, we functionalized Ti on the surface of Mg-Metal Organic Framework-74 (Mg-MOF-74) in order to enhance the hydrogen binding energy. For Ti adsorption sites on the Mg-MOF74, seven adsorption sites were considered, and we found that Ti binding energy ranges from 0.5-2.9 eV. Moreover, we put 1-3 H2 on the most stable Ti decorated site of Mg-MOF-74. Our results revealed that the hydrogen adsorption energies range from 0.51 to 2.43 eV/H2. Lastly, the hydrogen uptake of Ti-functionalized Mg-MOF-74 was evaluated by means of Ab initio Molecular Dynamics simulations. We found that the hydrogen capacities of this structure are 1.81, 1.79, and 1.29 wt% at 77, 150, and 298 K, respectively.

Summary

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