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Iron decorated - functionalized MOF for high-capacity hydrogen storage: First-principles calculations MOON-HYUN CHA, JISOON IHM, Department of Physics and Astronomy, Seoul National University — We perform electronic structure calculations for the Fe-decorated, OH-functionalized isoreticular metal organic framework 16 (IRMOF16) to investigate the hydrogen storage capacity. Because of the relatively strong Kubas interaction between Fe and H_2, hydrogen molecule can be adsorbed on the proposed MOF even at room temperature. The reversibly usable storage capacity under ambient conditions reaches 6.0 wt%. Fe has a much lower oxidation tendency than other metals (e.g., Ti, Ca, or Li) used for decorating backbone structures and therefore far more convenient in practical implementation. We also find that the spin flip, which comes from the competition between exchange field splitting and ligand field splitting, plays a significant role in the interaction between Fe and H_2.

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