

Abstract Submitted
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A comparative investigation of H₂ adsorption energy in Cd- and Zn-based metal organic framework-5 PORNJUK SREPUSHARAWOOT, Condensed Matter Theory Group, Dept. of Physics and Materials Science, Uppsala University, Sweden; Dept. of Physics, Khon Kaen University, Thailand, CARLOS MOYSÉS ARAÚJO, ANDEAS BLOMQUIST, RALPH SCHEICHER, CMT Group, Uppsala, RAJEEV AHUJA, CMT Group, Uppsala; Applied Materials Physics, Dept. of Materials and Engineering, Royal Institute of Technology (KTH), Stockholm, Sweden — Density functional theory has been used to study the physisorption energies of hydrogen at all possible adsorption sites near the metal oxide cluster in both Cd- and Zn-based Metal Organic Framework-5 (MOF-5). Three types of exchange- correlation functionals (LDA, GGA-PW91, and GGA-PBE) were compared. The binding for all adsorption sites in Cd-based MOF-5 was found to be generally stronger than in Zn-based MOF-5. In particular, the hydrogen adsorption energy at the secondary adsorption sites of Cd-based MOF-5 is increased by about 25% compared to Zn-based MOF-5. This result suggests that Cd-based MOF-5 might be better suited to store hydrogen at a given temperature than Zn-based MOF-5. See also: *J. Chem. Phys.* **129**, 164104 (2008).

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