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Theoretical investigation of hydrogen interaction in Covalent Organic Framework - 1 PORNJUK SREPUSHARAWOOT, RALPH H. SCHEICHER, C. MOYSÉS ARAÚJO, ANDREAS BLOMQVIST, RAJEEV AHUJA, Department of Physics and Materials Science, Uppsala University, SE-75121, Uppsala — Density functional theory (DFT) and second-order Møller-Plesset perturbation theory (MP2) are carried out to calculate the non-dissociative hydrogen adsorption energies of covalent organic framework-1 (COF-1). Our DFT results show that a hydrogen molecule prefers to adsorb on top of oxygen of boroxine (B_3O_3) ring and C—C bridge site of benzene ring when a single H_2 is interacting with the COF-1. Moreover, the trend of adsorption energy obtained from the DFT calculations is found to be in good agreement with the MP2 binding energy trend. However, hydrogen molecules prefer to trap on top of oxygen at B_3O_3 ring and carbon atom at C_6H_4 ring at high hydrogen loadings. By performing *ab initio* molecular dynamics simulations, we observed that H_2 molecules are able to stay at their initial adsorption sites due to blocking by occupancy of hydrogen molecules at the adsorption sites. (See also *J. Phys. Chem. C*, **113**, 8498 (2009))

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