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Energetics and dynamics of H_2 adsorbed in metal-organic frameworks from a van der Waals density functional approach[1] LINGZHU KONG, Rutgers University, NOUR NIJEM, UT Dallas, YONGGANG ZHAO, Rutgers, YVES J. CHABAL, UT Dallas, JING LI, DAVID C. LANGRETH, Rutgers — We performed van der Waals-density-functional calculations of the hydrogen adsorption in metal-orgnic frameworks.[2] The quantum dynamic behavior of the adsorbed dihydrogen is studied. The low-lying energy levels of the hindered rotational, frustrated translational and vibrational motions are calculated and compared with experimental inelastic neutron scattering and IR measurements. A consistent picture is obtained. Zero point energies due to the rotational and translational motions are estimated to be around 10 meV and 15 meV, respectively. The zero-point corrected binding energies agree with the measured isosteric heat of adsorption.

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[2]M. Dion et al. PRL 92,246401(2004); T. Thonhauser et al. PRB 76,125112(2007).

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