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Hydrogen spillover mechanism on covalent organic frameworks as investigated by DFT HONG ZHANG, Sichuan University, China — The hydrogen spillover mechanism, including the H chemisorption, diffusion, and H₂ associative desorption on the surface of COFs and H atoms migration from metal catalyst to COFs, have been studied via DFT. The results described herein show that each sp² C atom on COFs' surface can adsorb one H atom with the bond length d_{C-H} between 1.11 and 1.14 Å, and the up-down arrangement of the adsorbed H atoms is the most stable configuration. By counting the chemisorptions binding sites for these COFs, we predict the saturation storage densities. High hydrogen storage densities can be found that the gravimetric uptakes of COFs are in the range of 5.13 ~ 6.06 wt%. The CI-NEB calculations reveal that one H atom diffuse along C-C path on HHTP surface should overcome 1.41 ~ 2.16 eV energy barrier. We choose tetrahedral Pt₄ cluster and HHTP as the representative catalyst and substrate, respectively, to study the H migration from metal cluster to COFs.

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