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Theory of Hydrogen Storage: A New Strategy within Organometallic Chemistry

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As one of the most vigorous fields in modern chemistry, organometallic chemistry has made vast contributions to a broad variety of technological fields including catalysis, light emitters, molecular devices, liquid crystals, and even superconductivity. Here we show that organometallic chemistry in nanoscale could be the frontier in hydrogen storage. Our study is based on the notion that the 3d transition metal (TM) atoms are superb absorbers for H storage, as their empty d orbital can bind dihydrogen ligands (elongated but non-dissociated H_2) with high capacity at nearly ideal binding energy for reversible hydrogen storage. By embedding the TM atoms into a carbon-based nanostructures, high H capacity can be maintained. This presentation contains four parts. First, by comparing the conventional hydrogen storage media, e.g., metal hydrides and carbon-based materials, the general principles for designing hydrogen storage materials are outlined. Second, organometallic buckyballs are studied to demonstrate the novel strategy. The amount of H_2 adsorbed on a Sc-coated fullerene, $C_{48}B_{12}$ $[ScH]_{12}$, could approach 9 wt%, with binding energies of 30-40 kJ/mol. Third, the method is applied to the transition-metal carbide nanoparticles that have been synthesized experimentally. The similar non-dissociative H_2 binding is revealed in our calculation, thereby demonstrating the resilience of the overall mechanism. Moreover, a novel self-catalysis process is identified. In the fourth part, transition-metal functionalization of highly porous carbon-based materials is discussed heuristically to foresee macroscopic media for hydrogen storage. Finally follows the summary and discussion of the remaining challenges to practical hydrogen storage. Work in collaboration with A. C. Dillon, Y.-H. Kim, M. Heben & S. B. Zhang and supported by the U.S. DOE/EERE under contract No. DE-AC36-99GO10337.