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Hydrogen generation and storage over transition metal-decorated fullerenes and related materials LIPING HUANG, Department of Chemical and Biomolecular Engineering, North Carolina State University; Department of Physics, North Carolina State University, ERIK SANTISO, KEITH GUBBINS, Department of Chemical and Biomolecular Engineering, North Carolina State University, MARCO BUONGIORNO NARDELLI, Department of Physics, North Carolina State University; CSMD, Oak Ridge National Laboratory — Economical ways to generate and store hydrogen are crucial steps towards the hydrogen economy and fuel-cell technologies. By using first-principles density functional theory calculations, we found out that transition metal-decorated fullerenes and related materials can simultaneously dissociate small molecules like water to produce and store hydrogen. Hydrogen production from water will allow us to have a clean hydrogen economy by using renewable source rather than fossil fuels so that we can stop releasing carbon into the atmosphere. Our studies show that the bonding between transition metal and hydrogen is of a combination of chemical and physical adsorption, which is essential for reversible hydrogen uptake/release. Car-Parrinello molecular dynamics simulations demonstrate that these systems are stable and exhibit associative desorption of H_2 upon heating without breaking the bond between carbon and transition metal. This fulfills another requirement for reversible hydrogen storage.

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