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Optimization of metal dispersion and hydrogen adsorption strength in doped graphitic materials SEUNG-HOON JHI, GYUBONG KIM, Department of Physics, Pohang University of Science and Technology, NOEJUNG PARK, Department of Applied Phyiscs, Dankuk University, STEVEN LOUIE, Department of Physics, UC Berkeley, MARVIN COHEN, epartment of Physics, UC Berkeley — The non-covalent hydrogen binding on transition metal atoms dispersed on carbon clusters and graphene is studied with the use of the pseudopotential density functional method. It is found that the presence of acceptor-like states in the absorbents is essential for enhancing the metal-absorbent binding strength and for increasing the number of hydrogen molecules attached to the metal atoms. Particular configurations of boron or nitrogen substitutional doping are found to be very efficient for providing such states and thus enhancing storage capacity. Optimal doping conditions are suggested based on our calculations for the binding energy and ratio between metal and hydrogen molecules.

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