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Characterization and Control of the Barrier for Hydrogen Adsorption on Graphene[1] ALEJANDRO SUAREZ, Dept. of Physics, The Pennsylvania State University, LJUBISA RADOVIC, Dept. of Energy & Mineral Engineering, The Pennsylvania State University, JORGE SOFO, Dept. of Physics, The Pennsylvania State University — We study the chemisorption of atomic hydrogen on graphene. The barrier for chemisorption is about 0.21 eV. We explain the evolution of the partial density of states of the hydrogen and carbon atoms in graphene upon adsorption with a simple three-site Hubbard model. The barrier results from the competition between the pi-bonding between carbon atoms and the covalent bonding with hydrogen. With knowledge of the principles at play, we propose adjustments to the graphene plane which lower or eliminate this adsorption barrier. With a reduced barrier, formation of graphane can be facilitated, and applications for selective hydrogen desorption to create channels are discussed.

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