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Boron Doping Carbon Structures Using Decaborane? A Theoretical Study[1] CARLOS WEXLER, MATTHEW CONNOLLY, MATTHEW BECKNER, PETER PFEIFER, University of Missouri Physics Department, ALLIANCE FOR COLLABORATIVE RESEARCH IN ALTERNATIVE FUEL TECHNOLOGY COLLABORATION — Boron-doped carbon materials have been shown to improve hydrogen storage. Boron-doped activated carbons have been produced using a novel process involving the pyrolysis of a boron containing compound and subsequent high-temperature annealing. A model for the boron doping process based on a Langmuir isotherm is presented. A theoretical study of the interaction of the boron containing compound with the undoped carbon precursor will be presented. Ab-initio calculations of the potential energy surface and the Langmuir isotherm parameters derived from them are also presented. The theoretical study outlines the unique capabilities and limits of this doping procedure.

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