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Boron Doping of Activated Carbon MATTHEW CONNOLLY, ALEXANDER ST. JOHN, MATTHEW BECKNER, PETER PFEIFER, CARLOS WEXLER, University of Missouri — Efficient storage of hydrogen is one of the challenges to be solved for the H2-based fuelling systems. Carbon-based materials show promise, given their light weight, large surface areas and low cost. Unfortunately, the interaction of H2 and carbon, 5kJ/mol, is insufficient for room-temperature operation, the interaction energy for optimal delivery being ¿15kJ/mol. It has been proposed that boron doping of carbon materials could raise the binding energy of H2 to 12kJ/mol. However, the nature of the incorporation of boron into a carbon structure has not been studied in detail. Here, we address the energetics of boron incorporation into a carbon matrix via adsorption and decomposition of decaborane. First principles calculations demonstrate: (1) A strong adsorption of decaborane to carbon (70-80kJ/mol) resulting in easy incorporation of decaborane, sufficient for up to 10-20% B:C at low decaborane vapour pressures. (2) Identification that boron acts as an electron acceptor when incorporated substitutionally into a graphene-like material, as expected due to its valence. (3) The electrostatic field near the molecule is responsible for ca. 2/3 of the enhancement of the H2-adsorbent interaction. Supported by DOE DE-FG36-08GO18142, ACS-PRF 52696-ND5, and NSF 1069091.

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