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Energetics of Boron Doping of Carbon Pores[1] CARLOS WEXLER, ALEXANDER ST. JOHN, MATTHEW CONNOLLY, University of Missouri — Carbon-based materials show promise, given their light weight, large surface areas and low cost for storage of hydrogen and other gases, e.g., for energy applications. Alas, the interaction of H2 and carbon, 4-5kJ/mol, is insufficient for room-temperature operation. Boron doping of carbon materials could raise the binding energy of H2 to 12-15kJ/mol. The nature of the incorporation of boron into a carbon structure has not been studied so far. In this talk we will address the energetics of boron incorporation into a carbon matrix via adsorption and decomposition of decaborane by first principles calculations. These demonstrate: (a) 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. (b) Identification that boron acts as an electron acceptor when incorporated substitutionally into a graphene-like material, as expected due to its valence. (c) The electrostatic field near the molecule is responsible for ca. 2/3 of the enhancement of the H2-adsorbent interaction in aromatic compounds such as pyrene, coronene and ovalene.

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