Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Highly Selective CO_2/CH_4Gas Uptake by a Halogen-Decorated Borazine-Linked Polymer

THOMAS REICH, SWAYAMPRABHA BEHERA, KARL JACKSON, PURU JENA, HANI EL-KADERI, Virginia Commonwealth University — We report herein a synergistic approach that combines synthesis and characterization of a new borazine-linked polymer, BLP-10(Cl), and theoretical calculations based on density functional theory to investigate its performance in small gas storage and separation. We focus on the binding of H_2, CO_2, and CH_4. The choice of these gases is motivated by their impact on energy and the environment. Given the relatively small and similar kinetic diameter of the CH_4 and CO_2 molecules, their efficient separation remains a nontrivial task. In the case of a dihydrogen molecule interacting with the chlorinated borazine, we find the H_2 to be bound molecularly with a bond length of 0.75 Å and at a distance of 2.76 Å from the boron site. CO_2 and CH_4, on the other hand, interact with the central ring system of borazine at a distance of 3.12 Å and 3.33 Å respectively. The bond length between the carbon and oxygen atoms of CO_2 is 1.16 Å while the distance between the carbon and hydrogen of CH_4 is 1.10 Å. The binding affinities of all gases with the chlorinated borazine rings obtained from using the M06 exchange-correlation potential agree very well with experimental data collected form pure gas component isotherms. Theoretical investigations also indicate that all of the gas molecules preferentially interact with the borazine ring rather than the phenyl substituent of the nitrogen atoms which highlight the significance of including polarizable building blocks in adsorbent materials.

Swayamprabha Behera
Virginia Commonwealth University

Date submitted: 11 Nov 2011 Electronic form version 1.4