Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Hydrogen storage in a metal-organic-framework structure from a nonempirical van der Waals density functional approach[1] LINGZHU KONG, Rutgers, VALENTINO C. COOPER, Rutgers & ORNL, NOUR NIJEM, YVES J. CHABAL, UT Dallas, KUNHAO LI, JING LI, DAVID C. LANGRETH, Rutgers — Hydrogen adsorption in the metal-organic-framework structure $Zn_2(BDC)_2(TED)$ (BDC=benzenedicarboxylate; TED=triethylenediamine) is studied using a van der Waals-density-functional approach.[2] Two types of adsorbtion sites are located in the structure. The binding energies and the number of such sites are in good agreement with the values obtained from the experimental isotherms and isosteric heat of adsorption.[3] The stretching mode frequency of the adsorbed H_2 is calculated for various H–H bond orientations at the two positions. The frequency changes by approximately -30 cm^{-1} for the strongest binding direction at each of the two points, which is consistent with the measured infrared absorption band measured at 4120 cm^{-1} at room temperature and high pressures (300-800 psi).

[1]Supported by grants DOE-DE-FG02-08ER46491. Work by V.R.C. supported by NSF-DMR-0456937 at Rutgers and by DOE at ORNL.
[2]M. Dion et al., PRL **92**, 246401 (2004); T. Thonhauser et al., PRB **76**, 125112 (2007).
[3]J.Y. Lee et al., Adv. Func. Mater. **17**, 1255 (2007).

Lingzhu Kong
Rutgers

Date submitted: 01 Dec 2008 Electronic form version 1.4