Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Van der Waals density functional study of water binding in metal-organic frameworks KYUHO LEE, UC Berkeley; Molecular Foundry, LBNL, BEREND SMIT, UC Berkeley; LBNL, JEFFREY B. NEATON, Molecular Foundry, LBNL — Metal-organic frameworks (MOFs) are promising candidate materials for gas storage, gas separation and catalysis. However, MOFs are vulnerable to humid air and effective surface area drops dramatically on an exposure to water [1]. In this theoretical study, we investigate the interaction of single water molecule with MOF-74 on different binding sites by using van der Waals density functionals. We also explore how different type of metal cations affect the interaction.

[1] S. S. Kaye, A. Daily, O. M. Yaghi and J. R. Long, J. Am. Chem. Soc. **129**, 14176 (2007).

Kyuho Lee
UC Berkeley; Molecular Foundry, LBNL

Date submitted: 17 Nov 2012 Electronic form version 1.4