

Abstract Submitted  
for the NWS19 Meeting of  
The American Physical Society

**Adsorption Energies for Ten van der Waals Gases on a Zr-based Metal-Organic-Framework (MOF)**<sup>1</sup> OSCAR VILCHES, Dep. of Physics, U. of Washington, GRAEME VISSERS, WEI ZHANG, CHARLES CAMPBELL, Dep. of Chemistry, U. of Washington — MOFs are relatively novel crystalline, high controlled porosity, very large adsorption specific area materials designed for use as catalyst support and applications to scientific and applied problems. We present measurements of adsorption isotherms of ten gases (H<sub>2</sub>, D<sub>2</sub>, Ne, N<sub>2</sub>, Ar, CO, CH<sub>4</sub>, Kr, Xe and C<sub>2</sub>H<sub>6</sub>) over a wide range of the appropriate temperatures on a Zr-based MOF known as NU-1000 of specific area  $\approx 2600$  m<sup>2</sup>/gram. A first set of measurements<sup>1</sup> was used to calculate the differential heat of adsorption over the entire monolayer range. A second set emphasized the four central atoms/molecules in the series (N<sub>2</sub>, CO, Ar and CH<sub>4</sub>) for coverages under 0.1 monolayer for which density functional calculations (DFT) of the enthalpy of adsorption at zero coverage showed considerable variations. The DFT results indicated several strong adsorption sites with energy differences amongst them large enough for experimental observation. Our results show remarkable qualitative and semi-quantitative agreement with the DFT calculations assuming a sequential filling of sites, from strongest to weaker energies.<sup>2</sup> 1. W. Zhang et al., J. Am. Chem. Soc., 140, 328 (2018) 2. G. O. Vissers et al., J. Phys. Chem. C, (2019), in press.

<sup>1</sup>Work supported by DOE-OBES Chemical Sciences Division under grant DE-FG02-96ER14630 (G.O.V., W.Z., C. T. C.) and NSF DMR 1206208 (O.E.V).

Oscar Vilches  
University of Washington

Date submitted: 29 Mar 2019

Electronic form version 1.4