

Abstract Submitted  
for the MAR16 Meeting of  
The American Physical Society

**Noble gas adsorption in two-dimensional zeolites: a combined experimental and density functional theory study**<sup>1</sup> MENGGEN WANG, Stony Brook University, JIANQIANG ZHONG, JORGE ANIBAL BOSCOBOINIK, DEYU LU, Brookhaven National Laboratory — Zeolites are important industrial catalysts with porous three-dimensional structures. The catalytically active sites are located inside the pores, thus rendering them inaccessible for surface science measurements. We synthesized a two-dimensional (2D) zeolite model system, consisting of an (alumino)silicate bilayer weakly bound to a Ru (0001) surface. The 2D zeolite is suitable for surface science studies; it allows a detailed characterization of the atomic structure of the active site and interrogation of the model system during the catalytic reaction. As an initial step, we use Ar adsorption to obtain a better understanding of the atomic structure of the 2D zeolite. In addition, atomic level studies of rare gas adsorption and separation by zeolite are important for its potential application in nuclear waste sequestration. Experimental studies found that Ar atoms can be trapped inside the 2D-zeolite, raising an interesting question on whether Ar atoms are trapped inside the hexagonal prism nano-cages or at the interface between the (alumino)silicate bilayer and Ru(0001), or both. DFT calculations using van der Waals density functionals were carried out to determine the preferred Ar adsorption sites and the corresponding adsorption energies.

<sup>1</sup>This research used resources of the Center for Functional Nanomaterials, which is a U.S. DOE Office of Science Facility, at Brookhaven National Laboratory under Contract No. DE-SC0012704.

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Date submitted: 05 Nov 2015

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