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Thermodynamic, Modeling and Neutron Investigations of Cycloalkanes Adsorbed on MgO (100) and Graphite Basal Plane FATEMA WAHIDA, NICHOLAS STRANGE, JOHN Z. LARESE, Department of Chemistry, University of Tennessee, Knoxville, TN — Understanding the adsorption of molecules on solid surfaces is central to many scientific and technological challenges. Solid surfaces such as metal oxides, carbonaceous archetypes, porous silica, and metal organic frameworks currently represent significant components of nanomaterial research because of their widespread use in optoelectronics, separation chemistry, and catalysis. Understanding the interaction between adsorbed molecules and surfaces is a necessity for developing synthetic methods to produce materials with specific functional properties. An investigation of the effects of molecular and adsorbate symmetry is proposed in this study. The principal aim of this work is to identify the role of surface and molecular symmetry on the physicochemical properties of 2D layers of cyclic molecules adsorbed on metal oxide and semiconductor substrates. Initially our characterization will focus on the thermodynamic and microscopic structure and dynamics of cyclopentane and cyclohexane on the MgO (100) surface and graphite basal plane. In order to realize this goal adsorption isotherms, inelastic neutron scattering (INS) and molecular dynamics (MD) simulation studies will be performed to investigate the structure, dynamics and wetting properties.

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