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Thermodynamic and Modeling Study of Cyclopentane on MgO (100), hBN and Graphite Basal Plane FATEMA WAHIDA, NICHOLAS STRANGE, JOHN Z. LARESE, University of Tennessee, Knoxville — Investigation of the adsorption of cyclopentane on magnesium oxide (100), hexagonal boron nitride and the graphite basal plane was undertaken to explore the role of surface symmetry on the physicochemical properties. This is one portion of a broader study of 2D layers of cyclic organic molecules adsorbed on these scientifically and industrially important substrates. A series of high-resolution volumetric adsorption isotherms over the temperature range of 195-265K were measured on each of the substrates and used to calculate such thermodynamic properties as the heat of adsorption and isosteric heat, differential enthalpy, and differential entropy of adsorption during the layer growth process. The behavior of the two dimensional isothermal compressibility as a function of temperature and coverage was used to identify the locations of layering and potential phase transitions. To gain additional insight into the microscopic details of the adsorption process, classical molecular dynamics simulations were performed using a centralized force field (COMPASS) in tandem with thermodynamic experiments. The results of these modeling studies will be used to aid future quasi- and inelastic neutron scattering experiments aimed at exploring the rotational and translational diffusion and vibrational motion of the single and multilayer molecular films.

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