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5 to 6-fold symmetry transition and T-dependent stacking of Xe adsorbed on a quasicrystal surface WAHYU SETYAWAN, Duke University, STEFANO CURTAROLO, Duke University, RENEE DIEHL, Penn State University, NICOLA FERRALIS, Penn State University, R. A. TRASCA, Penn State University, MILTON COLE, Penn State University — The ordering of Xe films on an $Al_{73}Ni_{10}Co_{17}$ quasicrystals surface is studied using Grand Canonical Monte Carlo simulations with Lennard-Jones interatomic potentials and an empirical adsorption potential. Isotherms and layer density profiles show interesting phenomena. The study confirms the experimental layer-by-layer growth in the explored temperature (T) range (70-280K). By increasing the pressure at low temperatures (70-110K) the first layer, which forms following the 5-fold ordering of the substrate, evolves continuously assuming a 6-fold hexagonal symmetry before the condensation of the second layer. Thereafter, further layers have 6-fold symmetry. The 6-fold axes are aligned with the 5-fold axes of the quasicrystal, in agreement with experiment. However, at low T (70K) the layer stacking is ABC, consistent with fcc(111) experimental observations, while at higher T (160K) the stacking is AB, indicating a possible fcc to hcp transition of the adsorbate. Research supported in part by NSF.

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