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Computer simulations of the Adsorption of Xenon onto a C_{60} monolayer on Ag (111)[1] SILVINA GATICA, Howard University, MILTON COLE, RENEE DIEHL, Pennsylania State University — We performed Grand Canonical Monte Carlo simulations to study the adsorption of Xenon on a substrate composed of C_{60}molecules placed on top of a Ag(111) surface. The C_{60} molecules form a commensurate structure at a distance of 0.227 nm above the Ag surface. The interaction potential between the Xe atoms and the substrate has two contributions: from the C_{60} molecules and from the Ag atoms. In the simulations, the interaction with the Ag surface was computed using an *ab initio* van der Waals potential, varying as $1/d^3$. The interaction between the Xe atoms and each C_{60} molecule was computed using a potential previously developed by Hernandez et.al. (E. S. Hernandez, M. W. Cole and M. Boninsegni, "*Wetting of spherical surfaces by quantum fluids*", J. Low Temp. Phys. 134, 309-314 (2004)), who integrated the Lennard Jones interaction over the surface of a spherical buckyball. The total potential has especially attractive 3-fold sites, positioned 0.4 nm above the point between each three buckyballs. The low coverage uptake populates those sites, and then continues forming a monolayer. The adsorption isotherms show several steps, typical of substrates that have distinct adsorption sites. We compare the results with the experimental data.

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Silvina Gatica
Howard University

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