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Why viscosities of Ne and Kr monolayers are so different on the Pb(111) surface[1] RUQIAN WU, YANNING ZHANG, University of California, Irvine, V. BORTOLANI, Università di Modena e Reggio Emilia, Italy — Adsorption and segregation of Ne and Kr monolayers on the Pb(111) surface are examined through density functional calculations to understand the puzzling experimental observations of different tribological properties of these two rare gases. Theoretical results reveal weak but non-negligible interaction between rare gas and Pb(111), manifested as charge polarization and orbital intermixing. Because of its large atomic size, orbital polarizability and wave function extension, Kr binds with Pb(111) more strongly than does Ne. The activation energy of Kr segregation from the ground state hcp site to the metastable fcc site is 3.8 meV, substantially larger than that of Ne, 2.1 meV. This explains the drastic difference between the viscosities of Ne and Kr over Pb(111), observed at low temperatures using a quartz-crystal microbalance technique.

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