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Noble Gases on Metal Surfaces: New Insights on Adsorption Site Preference DE-LI CHEN, WISSAM AL-SAIDI, KARL JOHNSON, University of Pittsburgh — Experiments have previously found that noble gases (Kr, Xe) adsorb on low-coordination atop sites on several different metal surfaces, rather than on high-coordination hollow sites. This unexpected preference for low-coordination sites has been previously ascribed to reduced Pauli repulsion mostly due to exchange energy at the atop site, based on density functional theory calculations within the local density approximation (LDA). In contrast, our calculations using non-local van der Waals (vdW-DF) density functional show that site preference is due to a delicate balance between the electrostatics which favor the hollow site and kinetic energy which favors the atop site; exchange-correlation energies has a very little role. Moreover, we find, using LDA, GGA, and vdW-DF functionals, that the hollow site is a saddle point of index 1 or 2 on the 2-dimensional potential energy surface, while the atop site is the only true minimum. Therefore, the reason that hollow site occupation is not observed is that it is a transition state and so has a very short life-time. Our results show that the inclusion of non-local vdW interactions is crucial for obtaining results in quantitative agreement with experiments for adsorption energies, equilibrium distances, and vibrational energies.

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