Abstract Submitted
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Probe the Corrugation and Friction of Cu(111) toward Ne and Xe: First Principles Studies[1] YANNING ZHANG, University of California, Irvine, VIRGINIO BORTOLANI, Dipartimento di Fisica, Università di Modena e Reggio Emilia, RUQIAN WU, University of California, Irvine — The interaction between rare-gas (RG) and metal surface is typically described as the sum of two contributions: van der Waals attraction at large RG-metal distances, and Pauli repulsion at short distances. In the repulsive range, RG atoms can see a corrugated or anticorrugated potential surface, depending on the change of charge density profile of the surface atoms. The probe of the corrugation effects near the attractive part is also important since the corrugated or anticorrugated charge distribution at the surface can significantly change the physical properties of the whole system. In this letter, we show that also near the negative potential well of Ne and Xe monolayers on Cu(111), we can observe different surface corrugations: while the potential surface of Ne on Cu(111) is corrugated, it is anticorrugated for Xe/Cu(111). The analyses of electronic properties reveal that the weak hybridization of RG p- and substrate d-states is critical for the surface anticorrugation. Studies of the activation energies along sliding paths imply that Ne motion is much faster than Xe on Cu(111). Density functional calculations with self-consistent nonlocal van der Waals functional were used throughout our studies.

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