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Influence of Graphene Coating on the Adsorption and Tribology of Xeon Au(111) Substrate YANNING ZHANG, Chengdu Green Energy and Green Manufacturing Technology R&D Center, Sichuan, 620107, China, V. BORTOLANI, Dipartimento di Fisica, Università di Modena e Reggio Emilia, Via Campi 213/A,Modena, 41100 Italy, G. MISTURA, CNISM and Dipartimento di Fisica e Astronomia "G. Galilei," Università di Padova,Via Marzolo 8, Padova, 35131 Italy — The adsorption and tribological properties of graphene have received increasing attention for the further development of graphene-based coatings in applications. In thiswork, we performed first principles calculations with the inclusion of the nonlocal van der Waals correction to study the effect of graphene coating on the adsorption geometries, sliding frictions and electronic properties of Xe monolayer on the Au(111) substrate. Thecalculated activation energies indicate that Xe becomes movable on pure Au(111) surface at a temperature of around 30 K, whereas its motion can be activated only at a high temperature of ~ 50 K on graphene and on graphene-coated Au(111) substrates, in good agreement with recent experimental measurements by quartz crystal microbalance technique.

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