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Combined ab initio and classical molecular dynamics simulations of the tribological properties of rare gas monolayers sliding on metal surfaces MARIA CLELIA RIGHI, CNR-INFM S3 National Research Center, Via Campi 213/a Modena, Italy, MAURO FERRARIO, Universita' di Modena e Reggio Emilia — Progress in the ability of understanding tribological properties in adsorbed film systems is of paramount importance to unravel fundamental issues in the emerging field of nanoscale science and technology. Many extensive studies have used a quartz-crystal microbalance (QCM) to measure the friction between adsorbed rare gas monolayers and metal substrates. In this work, we report a theoretical investigation of the tribological behavior of different rare gas-metal adsorbate systems, namely, Ar, Kr, Xe on Cu(111), and Xe on Ag(111), based on combined *ab initio* and classical molecular dynamics simulations. The frictional properties are analyzed in details as a function of system temperature, presence of interlayer defects, and load. The numerical simulations suggest that the simultaneous presence of thermal effects and of interlayer defects, lowering significantly the activation energy barrier, causes a considerable reduction of the static friction threshold. An unexpected dependence on load is also predicted. In particular, we show that friction of anticorrugating systems can be dramatically decreased by applying an external load [1]. The counterintuitive behavior that deviates from the macroscopic Amonton law is dictated by quantum mechanical effects that induce a transformation from anticorrugation to corrugation in the near-surface region. [1] M. C. Righi and M. Ferrario, Phys. Rev. Lett. **99**, 176101 (2007).

Maria Clelia Righi
CNR-INFM S3 National Research Center, Via Campi 213/a Modena, Italy

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