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Motion of Sb nanoparticles on HOPG: simulation study of frictionless behavior[1] IVAN STICH, JAN BRNDIAR, ROBERT TURANSKY, Inst. Phys., Slovak Acad. Sci. — Using DFT total energy techniques adapted to accommodate van der Waals dispersion forces, we have simulated the behavior of the recently studied motion Sb nanoparticles on HOPG surface with the quest to elucidate the experimentally observed frictional duality [1, 2]. Both frictionless and "normal" behavior, which scales with apparent contact area was identified experimentally. Several different nanoparticle geometries, including atoms, small to medium size clusters, and surfaces were included in the simulations. The Sb-HOPG interface is found to be primarily van der Waals bonded. From the simulations the frictionless behavior can only be accounted for by a self-lubricity mechanism. Therein the smallest structurally stable Sb tetrahedra, attached to the contact plane of the Sb nanoparticle, yield essentially uncorrugated potential energy surfaces and hence, frictionless sliding over HOPG. [1] D. Dietzel, Phys. Rev. Lett. **101**, 125505 (2008). [2] A. Schirmeisen, U.D. Schwarz, ChemPhysChem **10**, 2373 (2009).

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