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Does rotational melting make molecular surfaces more slippery?[1]
ANDREA BENASSI, CARLO PIGNEDOLI, DANIELE PASSERONE, Swiss Federal Laboratories for Materials Science and Technology, EMPA, ANDREA VANOSSI, CNR-IOM Democritos and SISSA, Trieste, Italy, ERIO TOSATTI, SISSA, ICTP, and CNR-IOM Democritos, Trieste, Italy — Crystals made up of spherical, weakly interacting molecules generally exhibit a phase transition between a low temperature ordered phase and a plastic phase, where the rotational order is thermally lost. In C_{60} fullerene, the transition takes place at T_r=260K in bulk, initiating at a lower temperature at a (111)surface. We explore by MD simulations whether a slider should experience a change of friction on that surface in correspondence with the phase transition. Modeling the slider as a C_{60} flake attached to a sliding tip, we obtain a response dependent on the orientation and the angular compliance of the flake. An orientation angle commensurate with the C_{60} surface yields a large adhesion and friction, both dropping by only about 20% at the plastic transition. An incommensurate angle yields both adhesion and friction a factor 2 smaller and relatively unaffected by the transition. Finally, a sliding flake with an incommensurate angle but a compliant orientation offers the possibility of a very different sliding behavior, remaining incommensurate with very low adhesion/friction above T_r, but jumping to a commensurate angle with high adhesion/friction below T_r. This third possibility might have been realized in the AFM experiment by Liang et al.(PRL 2003).

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