Exfoliation of graphene through activation of superlubricity

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Superlubricity is the physical phenomenon where friction drastically decreases between two crystalline surfaces in incommensurate contact. In layered materials such as graphite, superlubricity can be activated by rotation of the layers with respect to each other. Through classical molecular dynamics (MD) simulations, we show that the compression of few-layered graphene on hydrogen-passivated silicon substrates can activate coupling between the sliding and rotation of the graphite flakes in incommensurate contact with the substrate. This coupling causes the graphene flakes to reorient themselves to more stable states, leading to thinning of these flakes to produce single-layer graphene on the substrates. This behavior has been observed in simulations for silicon substrates of both (111) and (110) surface orientation. In contrast, a perfectly smooth Lennard-Jones potential wall is incapable of activating such a phenomenon.

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