Study of Ultra-low Friction in Two-Dimensional Materials using Density-Functional Theory

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The superior lubrication capabilities of two-dimensional crystalline materials such as graphene, hexagonal boron nitride (h-BN), and molybdenum disulfide (MoS_2) have been well known for many years. It is generally accepted that superlubricity in these materials is due to misalignment of the surfaces in contact, known as incommensurability. However, recent studies using molecular dynamics simulations have demonstrated that incommensurability may not be a requirement for the superlubric behavior in MoS_2 [Comp. Mater. Sci. 163, 17 (2019)]. In this light, a detailed analysis of friction in commensurate, and structurally incommensurate 2D materials is presented. In particular, we investigate superlubricity in bilayer graphene, h-BN, MoS_2, and the novel material blue phosphorene using dispersion-corrected density-functional theory. For each material, interlayer sliding has been modeled, the associated energy barriers computed, and the corresponding potential energy surfaces plotted. We have considered rotation angles of 0° for the commensurate case, and 21.79°, 32.20° and, 13.17° for the incommensurate counterparts. Finally, the coefficients of friction for each configuration have been reported. These coefficients remain 1-2 orders of magnitude lower for the incommensurate structures. Provided the rotation barriers can be overcome, superlubricity is expected to occur in the rotated structures.