Friction between bilayer of 2D crystalline nanomaterials: graphene–graphene, graphene–boron nitride, and boron nitride–boron nitride.

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ABSTRACT

We performed molecular dynamics simulation for comprehensive analysis of friction between bilayer of 2D crystalline nanomaterials: Graphene–Graphene, Graphene–Boron Nitride (BN) and BN–BN. For Graphene–Graphene and BN–BN friction, we investigated the effect of defect (vacancy, stone-wale) and surface functionalization by hydrogen. Our results show that presence of defect influences the frictional properties. Moreover, hydrogen functionalization will increase the friction because of the increase of surface roughness. We investigated the variation of frictional force with surface functionalization. The last model considered the friction between Graphene–BN. The interface between Graphene–BN substrate plays a crucial role in application of nanodevices. We analyzed the energy landscape, evolution of Moire pattern and frictional force between sheets for various conditions. This comprehensive study will help understand deeply the mechanics of friction of 2D crystalline nanomaterials.