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Ab initio study of friction of graphene flake on graphene/graphite or SiC surface¹ OGUZ GULSEREN, Bilkent University, CEREN TAYRAN, Gazi University, CEREN SIBEL SAYIN, Bilkent University — Recently, the rich dynamics of graphene flake on graphite or SiC surfaces are revealed from atomic force microscopy experiments. The studies toward to the understanding of microscopic origin of friction are getting a lot of attention. Despite the several studies of these systems using molecular dynamics methods, density functional theory based investigations are limited because of the huge system sizes. In this study, we investigated the frictional force on graphene flake on graphite or SiC surfaces from pseudopotential plane-wave calculations based on density functional theory. In both cases, graphene flake (24 C) on graphite or SiC surface, bilayer flake is introduced by freezing the top layer as well as the bottom layer of the surface slab. After fixing the load with these frozen layers, we checked the relative motion of the flake over the surface. A minimum energy is reached when the flake is moved on graphene to attain AB stacking. We also conclude that edge reconstruction because of the finite size of the flake is very critical for frictional properties of the flake; therefore the saturation of dangling bonds with hydrogen is also addressed. Not only the symmetric configurations remaining parameter space is extensively studied. Supported by TUBITAK Project No: 114F162.

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