

Abstract Submitted
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Ab Initio Investigation of Frictional Properties of Graphene on SiC Surfaces¹ CEREN SAYIN, OĞUZ GÜLSEREN, Bilkent Univ — The exact origin and nature of various nanotribological observations on graphene such as dependence of friction on layer thickness, direction and surface morphology are yet to be fully understood. In this talk, we report on the frictional properties of graphene on 4H-SiC{0001} surfaces obtained from first principles calculations. We investigate sliding of graphene layers of various thickness along different directions on both the Si- and C-terminated faces including van-der Waals interactions. We observe that upon sliding under certain conditions, the interaction between the surface and graphene layers alternates between van-der Waals and covalent forces which dramatically affects friction. We examine the relation of frictional force to applied normal load, small out-of-plane geometric deformations of graphene and electronic structure of the systems.

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