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Theory of nanoscale friction on chemically modified graphene JAE-HYEON KO, YONG-HYUN KIM, Graduate School of Nanoscience and Technology, KAIST — Recently, it is known from FFM experiments that friction force on graphene is significantly increased by chemical modification such as hydrogenation, oxidization, and fluorination, whereas adhesion properties are altered marginally [1]. A novel nanotribological theory on two-dimensional materials is proposed on the basis of experimental results and first-principles density-functional theory (DFT) calculations. The proposed theory indicates that the total lateral stiffness that is the proportional constant of friction force is mostly associated with the out-of-plane bending stiffness of two-dimensional materials. This contrasts to the case of three-dimensional materials, in which the shear strength of materials determines nanoscale friction. We will discuss details of DFT calculations and how to generalize the current theory to three dimensional materials. [1] S. Kwon, J.-H. Ko, K.-J. Jeon, Y.-H. Kim and J. Y. Park, Nano Lett., dx.doi.org/10.1021/nl204019k (2012).

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