**A Simple Method to Calculate the Exfoliation Energies of Layered Materials**

Jong Hyun Jung,1 Cheol-Hwan Park,1,\* and Jisoon Ihm2

*1 Department of Physics and Astronomy, Seoul National University, Seoul 08826, South Korea*

*2 Department of Physics, Pohang University of Science and Technology, Pohang 37673, South Korea*

\* E-mail: cheolhwan@snu.ac.kr

The exfoliation energy, the energy required to peel off an atomic layer from the surface of a bulk material, is of fundamental importance in the science and engineering of layered materials. Traditionally, the exfoliation energy has been obtained from first-principles by calculating the difference in the energy between (i) a slab of *N* layers (*N* 1) and (ii) a slab of *N* – 1 layers plus a layer separated from the slab. Here, we prove that the exfoliation energy can be obtained *exactly* as the difference between the energy of a bulk material (per atomic layer) and that of an isolated single layer [1]. The proposed method is (i) tremendously lower in computational cost than the traditional approach because it does not require calculations on thick slabs, and (ii) still valid even if there is a surface reconstruction of any kind. Moreover, the method is (iii) capable of taking into account the relaxation of the exfoliated single layer, and (iv) easily combined with many-body computational methods. As a proof of principles, we calculate the exfoliation energies of graphene, hexagonal boron nitride, MoS2, and phosphorene using density-functional theory.



1. J. H. Jung, C.-H. Park, and J. Ihm, Nano Lett. **18**, 2759 (2018).