

Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Poisson's Ratio of Layered Two-dimensional Crystals SUNGJONG WOO, HEE CHUL PARK, YOUNG-WOO SON, Korea Institute for Advanced Study — We have investigated the elastic properties of multilayered graphene as well as h-BN and MoS₂ using a first-principles approach with up-to-date nonlocal exchange-correlation energy functional. Our analysis shows that the Poisson's ratios of multilayered graphene, h-BN and MoS₂ along out-of-plane direction are negative, near zero and positive, respectively, spanning all possibilities for sign of the ratios. While the in-plane Poisson's ratios are positive regardless of their disparate electronic and structural properties, the characteristic interlayer interactions as well as atomic stacking structures are shown to determine the sign of their out-of-plane ratios, highlighting their intertwined nature between elastic and electronic properties.

Sungjong Woo
Korea Institute for Advanced Study

Date submitted: 14 Nov 2014

Electronic form version 1.4