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Effects of static charging and exfoliation of layered crystals MEHMET TOPSAKAL, SALIM CIRACI, UNAM-Institute of Materials Science and Nanotechnology — Using first-principle plane wave method we investigate the effects of static charging on structural, electronic and magnetic properties of suspended, single layer graphene, graphane, fluorographene, BN and MoS(2) in honeycomb structure. The limitations of periodic boundary conditions in the treatment of charged layers are clarified. Upon positive charging the band gaps between the conduction and valence bands increase, but the single layer nanostructures become metallic owing to the Fermi level dipping below the maximum of valence band. Moreover, their bond lengths increase leading to phonon softening. As a result, the frequencies of Raman active modes are lowered. High level of positive charging leads to structural instabilities in single layer nanostructures, since their specific phonon modes attain imaginary frequencies. Similarly, excess positive charge is accumulated at the outermost layers of metallized BN and MoS(2) sheets comprising a few layers. Once the charging exceeds a threshold value the outermost layers are exfoliated. Charge relocation and repulsive force generation are in compliance with classical theories.

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