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Equation of state for a 2D system

We have described a simple theoretical model of an equation of state (EOS) for a two-dimensional system. The goal was to give a clear description of the interplay between hydrostatic change in surface area and the two dimensional in-plane pressure (F). Of interest from this described EOS, was the measure a material's resilience to isotropic stretching (γ) that can in principle be viewed as the layer modulus. To this date, few attempts have been made to obtain accurately the layer modulus of 2D systems. We studied using density functional theory as implemented in the {\sc SIESTA} computer code, a number of monolayer systems; graphene, boronitrene, dichalchogenides and janus chalcogenides. The results found out in this study showed that of the above honeycomb structures, graphene was the most resilient to stretching with a value of $\gamma_C = 206.6\ N/m$ followed by boronitrene $\gamma_{BN} = 177.3\ N/m$. The layer modulus of the dichalcogenides and janus chalcogenides was seen to be competing but not as large as that of graphene or boronitrene. Apart from the layer modulus, we were also able to use the EOS to predict isotropic intrinsic strength of the listed systems. It was observed that the instrinsic stress was proportional to the layer modulus. This project does not just satisfy our knowledge thirst but can also be used by experimental groups in fabricating hard 2D materials.

Keywords

EOS, first-principles, Density functional theory, layer modulus.

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