

Abstract Submitted
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Long-range interaction of anisotropic systems¹ JUN-YI ZHANG, UDO SCHWINGENSCHLÖGL, Division of Physical Science & Engineering, King Abdullah University of Science and Technology — The first-order electrostatic interaction energy between two far-apart anisotropic atoms depends not only on the distance between them but also on their relative orientation, according to Rayleigh Schrödinger perturbation theory. Using the first-order interaction energy and the continuum model, we study the long-range interaction between a pair of parallel graphene sheets. The asymptotic form of the obtained potential density, $\varepsilon(D) \propto -D^{-3} - O(D^{-4})$, is consistent with the random phase approximation and Lifshitz theory. Accordingly, neglectance of the anisotropy, especially the nonzero first-order interaction energy, is the reason that the widely used Lennard-Jones potential approach and dispersion-corrections in density functional theory give a wrong asymptotic form, $\varepsilon(D) \propto -D^{-4}$.

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