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A method of numerical evaluation of some physical properties of Van der Waals structures

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A simple method of fast numerical modeling, convenient for accurate estimation of a set of physical properties of graphite and other similar van der Waals homo/heterostructures is proposed. It reproduces experimental values of compressibility along c-axis under broad pressure range, Raman frequencies for bulk shear and breathing modes under pressure, layer binding energies. It is argued that anisotropic Kolmogorov-Crespi and Lebedeva equations of interlayer potential are best suited for accurate self-consistent description. The method of computation we use is based on observation that in graphite there are two types of ordering of atoms between two neighboring planes, as shown in Figure 1. Atoms are formed in equi-distant rings. The radius of these rings is known analytically. We do not know a method to predict theoretically the number of atoms in rings. These numbers can however be found by using algorithms that analyze the structure of single plane of graphene, and can be tabulated. We sum contribution to potential energy of inter-plane interaction by adding contributions from rings. The method is found to converge quickly with adding larger and larger rings. Once we know potential energy of a structure of planes, we are able to compute its several physical properties, as for instance compressibility of graphite along c-axis, as shown in Figure 1.B.

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