π-electrons of Multi-layer Graphene Under Compression

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We aim to understand the behaviour of the π-electrons of multi-layer graphene under compression by quantifying its effect on various properties of graphene. First, we noticed the difference in reported values of the shift rates with pressure of the graphite two in-line antiphase vibrational frequencies E_{1u} (two graphene planes vibrate in-phase) and E_{2g} (out-of-phase, the GM). The commonly-used two dimensional analysis was not able to explain this. We introduced a new parameter to quantify the effect of the compression of π-electrons into the sp^2 network to change the in-plane bond stiffness. Then the main effect of the π-electrons is to determine the interlayer interaction between graphene layers, of which we used frequencies of interlayer phonon modes, the shear mode and layer breathing mode as measures. We employed a linear chain model and expand the force constant in terms of the interlayer spacing. Finally, we compared Bernal-stacking to A-A stacking. We quantify the amount of electrons squeezed through the sp^2 planes and shifts of phonon frequencies under compression for these two stacking types.