**Computation of Intrinsic Mechanical Properties of Double Layer Graphene**

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Until the second trimester of the late century only two ordered forms of carbon were known to scientists, namely diamond, with its perfect crystal structure, and graphite, also crystalline but black and flaky and not at all transparent. Besides those ordered forms, also coal, coke, soot, lampblack, and the many kinds of charcoal were known. The graphite structure reflects its properties, since it is made up of sheets of carbon atoms arranged in a hexagonal lattice, like a honeycomb of fused benzene rings, and with weak bonding between adjacent sheets. This means that graphite easily forms flakes where the sheets can slide over each other, providing use of graphite as a lubricant, and resulting good electrical conductivity. But it is only in 2007 that researchers in Manchester found a way to mechanically peel single two-dimensional sheets from three-dimensional graphite crystals[1]. Graphene is the name given to this flat monolayer of carbon atoms tightly packed into a two-dimensional honeycomb lattice.

Since the first experimental analysis[1], graphene has recently gained significant attention. In particular, its excellent mechanical properties are an important advantage for the practical applications of graphene. These mechanical properties have extensively been investigated, and in particular, the Young's Modulus has been predicted using a range of experimental and theoretical approaches.

On the experimental side, by ultrasonic, sonic resonance, and static test methods, Blakslee *et. al.*[2] reported a Young's modulus of 1.06 TPa for bulk pyrolytic graphite, which has been highly ordered by annealing under compressive stress. Frank *et al.*[3] measured the modulus for a stack of graphene sheets (less than five layers) to be 0.5 TPa using an atomic force microscope. More recently, by nano-indenting the centre of a free-standing monolayer graphene membrane with an atomic force microscope, Lee *et al.*[4] measured the Young's modulus as 1.0 TPa, assuming the thickness of graphene to be 0.335 nm.

Many theoretical and computational studies have also been performed to investigate the mechanical properties of graphene, for example, the pioneering study by Van Lier *et al.*[5], using super-molecular approach. There are numerous theoretical studies using a super-molecular approach, to calculate mechanical properties, however the number of infinite (periodic) calculations is very scarce[6]. Stress-strain curves are seldom reported, and other mechanical properties for example bending modulus were not investigated up to now.

In this study, the Young's and bending moduli of single and double layer graphene have been theoretically investigated using Periodic Boundary Condition (PBC) Density Functional Theory (DFT) with the PBE, HSEh1PBE, and M06L functionals in conjunction with the 6-31G* and the 3-21G basis sets. The unit-cell size and shape dependence as well as the directional dependencies of the mechanical properties have been also investigated. The calculated stretching and bending strain-stress curves are also reported (see figures).

**References**

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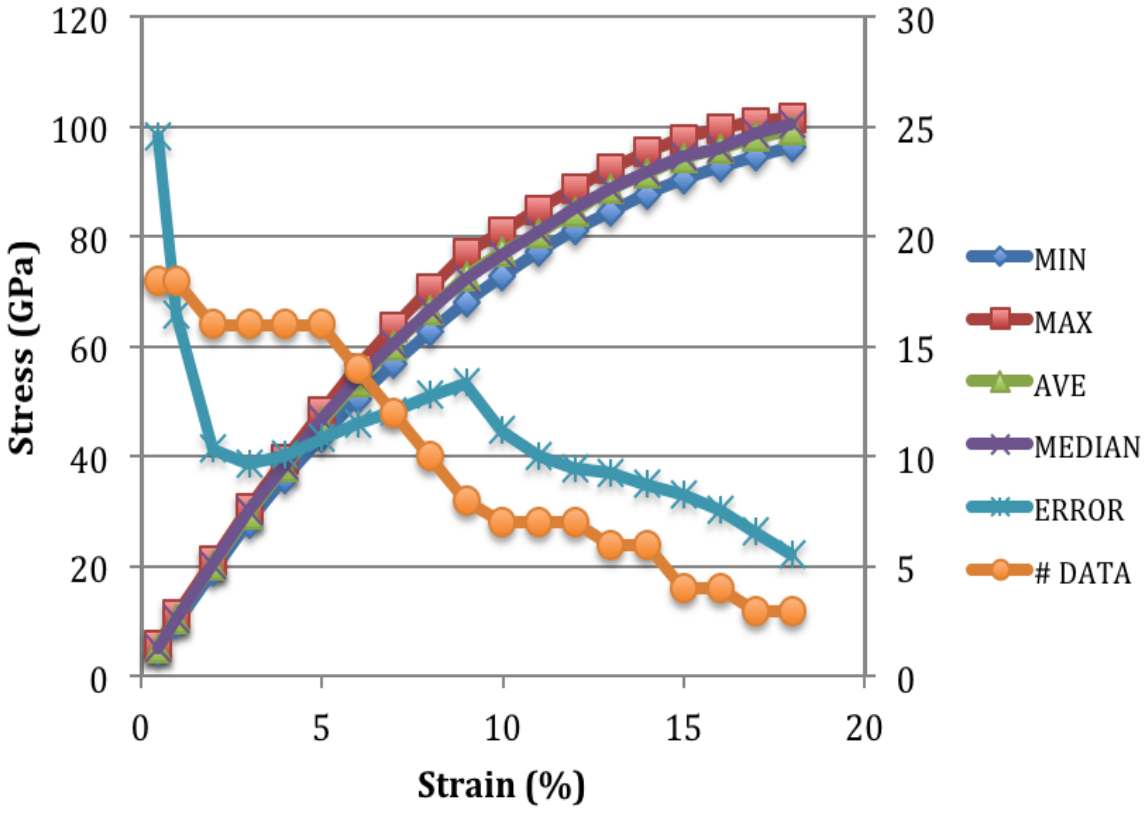
**Figure**




*Stress-Strain curves for double-layer graphene, using all employed methods (only 3-21G basis set). Both the errors between the minimum and maximum in percentage and the number of different levels of theoretical calculations (# DATA) are displayed on the right axis.*