Computational Study of 3D Structures of Pillared Graphene

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Molecularly pillared graphene (MPG) consists of layers of graphene, which are interconnected via organic molecules (pillars) with functional groups. The numerous combinations of pillars and functional groups in MPGs, present high possibility for creating materials with tuneable properties and enhanced characteristics [1-3]. The purpose of this computational study is to design MPGs by employing periodic boundary conditions, within the frameworks of density functional (DFT) and tight binding (TB) levels of theory, and to investigate the ability of tuning its properties by employing different functional groups. The computations were performed for two different unit cells of bilayer graphene oxide interconnected with 1,4-benzenediamine and 1,4-benzenedithiol, respectively. Initially, we optimized the pillars using the PBE functional [4] with the Gaussian package [5]. Secondly, we performed geometry and cell optimizations simultaneously, by employing different computational methods. Firstly, we employed the GFN1-xTB [6,7] method using the CP2K code [8]. The obtained structures were re-optimized with the PBE functional using the Quantum Espresso package [9]. The PBE computations were repeated by including Grimme's dispersion correction D3. The Density of states (DOS) of the optimized geometries were examined in all cases, with the Quantum Espresso package.

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Figures

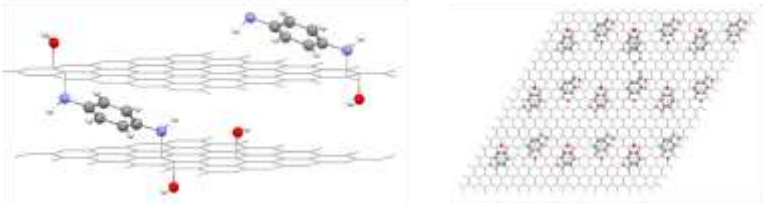

Figure 1: Unit cell with 1,4-benzenediamine (left) and supercell (right)

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