SimVacGraph – Magnetism of bilayer graphene with vacancies

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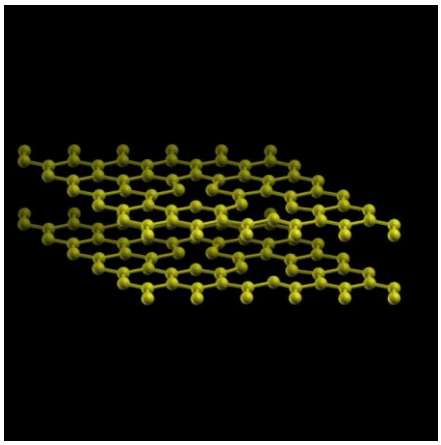

Figure 1: AA bilayer stack: the distance between the sheets was initially set to 3.3 Å

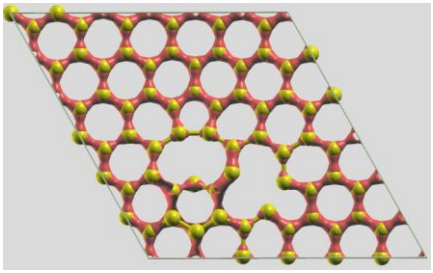

Figure 2: The top view of the iso-surface distribution of the electron density in AA bilayer graphene with vacancies on top of each other.

❖ Description of the problem

The bilayer graphene exists in three modifications: AA, AB (or Bernal phase), and twisted bilayer. The simplest form is the AA bilayer - each carbon atom of the second layer is placed exactly above the corresponding atom of the first graphene layer. Monoatomic vacancies in AA bilayer graphene were computationally studied to monitor the possibility to switch between nonmagnetic, antiferromagnetic and ferrimagnetic states. The importance of these transitions is related to technological applications of bilayer graphene and to fundamental understanding of the symmetry breaking in finite-size systems. We have implemented the spin-polarized Density Functional Theory in the version of the Quantum Espresso 5.4.0 that contains programs for electronic structure calculations and density functional perturbation theory, using a plane-wave basis set and pseudopotentials.

The team from Sofia University works on the project in cooperation with a team from the high-performance computing laboratory at the Sofia Tech Park, [1].

❖ Use of HPC Infrastructure (How HPC makes the difference)

The HPC clusters NESTUM [1] and PhysOn [2] were used to obtain the simulation results. The PhysOn cluster is located in the HPC laboratory of he Faculty of physics, Sofia University. Both NESTUM and PhysOn clusters are maintained via funding from the National Roadmap for Research Infrastructures (NRRI).

The results presented here were obtained in parallel computations on 5 nodes, with 24-cores each, designed with 2 pcs. 64-bit 6-core Intel Xeon® E5-2650v4 processors, 94 GiB shared memory, InfiniBand controller with a throughput of 56 Gbps

❖ Results and Future Work

The spin density is non-uniformly distributed among the atoms around the vacancies and the nearest neighbors contributing to non-zaro magnetic moment of AA bilayer graphene. The Fermi level of the system is 1.5243 eV and there is an opening in the vicinity of the Fermi level, which classifies this stack as a semiconductor. The reduction of the magnetic moment due to the interlayer bonding is an important result, which opens the possibility of various technological applications.
In the future the adsorption ability of bilayer graphene with double-vacancies will be studied.

1. http://hpc-lab.sofiatech.bg/home/
2. http://physon.phys.uni-sofia.bg