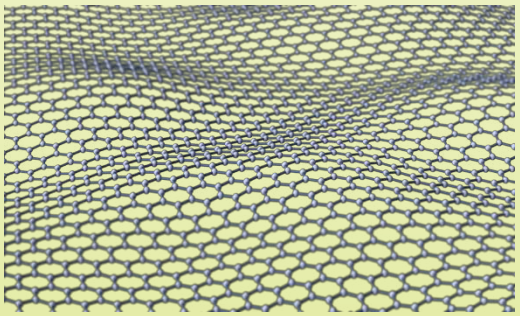
Conclusions

- GDQs are potential candidates for QIP thanks to their properties which ensure the highest coherence time for electron spin confined inside the dot.
- Nevertheless, defects or impurities can introduce decoherence, resulting in possible loss of information.
- Vacancy, the simplest point defect, breaks the symmetry of graphene system, giving rise to localized states which provide a magnetic moment different from zero. Magnitude depends on defect concentration.
- Hydrogen hybridizes locally the system and gives rise to a magnetic moment. Furthermore, it enhances the spin-orbit coupling of about 3 order of magnitude with respect to the intrinsic spin-orbit interaction for graphene. Interactions between 2 H follow the Lieb's scheme.
- Among B, N, and O, the only one which returns a magnetic ground state is N. The magnitude of the magnetic moment may depend on adatom-concentration. O seems to be the least dangerous element for the purpose of QIP.

Acknowledgments

All the *ab initio* simulations have been performed using Quantum Espresso, a parallelized Density Functional Theory code developed at SISSA, Trieste.

QUANTUMESPRESSO



Thanks are due to the Jülich Forschungzentrum (Germany) and to the RWTH, Aachen (Germany) for computational time.

Thanks to the research group of Prof. Mazzarello for their availability and for supporting me in the development of my work.

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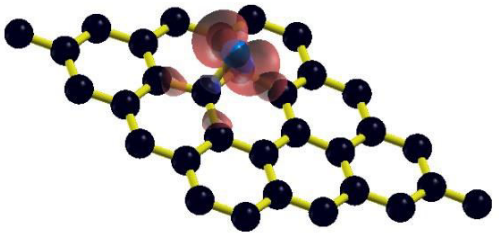

DEFECT-INDUCED MAGNETISM IN GRAPHENE: AN *AB INITIO* STUDY

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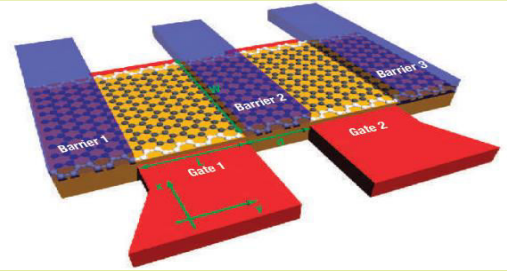
Anno Accademico 2014/2015

Introduction

Some potential applications in **Quantum Information Processing** (QIP) have been proposed for **C-based materials**, in particular for **graphene system**. Electron spin is a promising candidate for a **solid-state qubit.**

In principle, one can exploit the absence of **hyperfine interaction**, small **spin-orbit interaction** and energy spectrum of **Graphene Quantum Dot (GQD)** to get an efficient system for quantum computation, preserving important features such as a **long spin-coherence time**.

However, **defects** in the structure, **impurities** and **edge states** can be **source of decoherence**, providing a **loss of quantum information**.



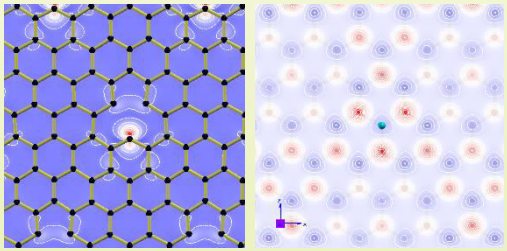
Purposes

Our work is aimed at achieving a better understanding of the effects provided by impurities on graphene,.

- ***Ab initio* spin-polarized simulations** performed to **resolve magnetism in defective graphene**.
- Analysis of effects produced by defects and by **interactions of adatom on graphene surface**.

Vacancy-type defect *vs.* hydrogen-adatom impurities

Vacancy-defects and hydrogen adatoms both give rise to **a breaking of graphene *bipartite lattice* symmetry**, promoting localized states occupied by unpaired electrons and providing a magnetic moment.



Results for vacancy:

- Removal of C → Three dangling bonds.
- Two of them saturate forming a covalent bond, the 3°-one unsaturated gives rise to 1 μ_B/cell, where the quasi localized p_z state provides a fractional magnetic moment → saturation value: 1.5 μ_B/cell
- **Vacancies tend to reconstruct** → the magnetic moment **depends on defect concentration.**

Results for hydrogen:

- sp^3-hybridization of C in top-adsorption site (most stable) → strong interaction.
- **Constant magnetic moment: 1 μ_B/cell.**
- **Enhancement** of spin-orbit interaction.
- According to Lieb's theorem: 2 H in the same sublattice→ ferromagnetic order, where in different sublattice→ antiferromagnetic one is more stable (the last one, dependently by the distance).

Boron-, Nitrogen-, and Oxygen-graphene systems: magnetic properties

Evaluation of adsorption energies for different sites returns the *bridge-site* as the most stable configuration for B,N and O.

Results:

Boron

- **Weak interaction** with graphene.
- **Ionic bonding** with **charge transfer** from B to graphene → **n-doping.**
- **Non-magnetic ground state**.

Nitrogen

- Relatively strong interaction with graphene surface → **covalent bonding**.
- **Magnetic ground state** → ~ 1 μ_B/cell
- The magnitude of **magnetic moment** shows a **dependence** on the **adatoms concentration** (∝ cell size) → the biggest cell shows ~ 0.74 μ_B/adatom.
- **Interaction between 2 N** develops always a **ferromagnetic order** (at 0° K).

Oxygen

- **Similar interaction of N**, but **with non-magnetic ground-state**.