Magnetic moments in a graphene sheet with vacancies generated by proton-beam bombardment

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20th international conference on
Nanoscience and Nanotechnology, NANO’2018
Sofia, 8-10.11.2018, Bulgarian Academy of Sciences

Layout

- Vacancies in graphene due to beam bombardment
- Beams of electrons, protons, neutrons, ions generate vacancies in graphene with different properties

Interest

Physical understanding of the interaction **between energetic particles and suspended graphene** can practically lead to reproducible and efficient **pattern generation** of unprecedentedly small features on 2D materials by design, manifested by perforation of sub-5-nm pore arrays.

Interest

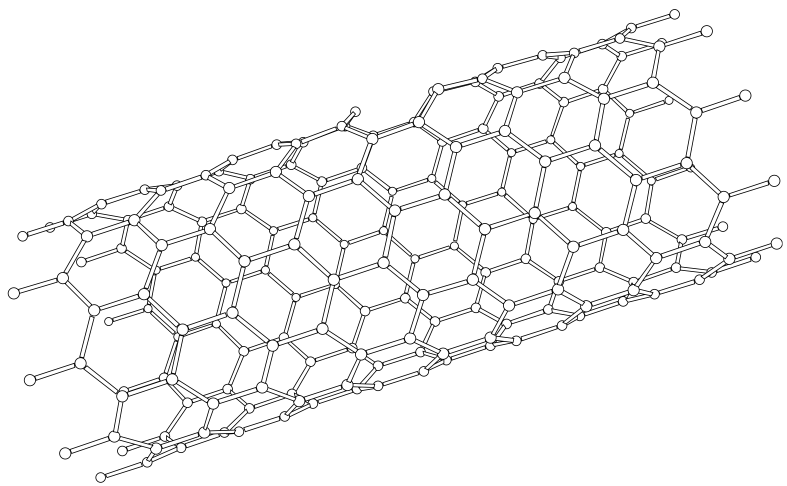
Potential graphene-based technology is proposed for various applications including ultimately permeable membranes and flexible electronics

The evolution of the electrical properties and quality of supported or sandwiched graphene subject to ion irradiation has been investigated, all assuring that graphene can be patterned by energetic ion irradiation.

Defective graphene study

A long journey started in 2007 with single carbon nanotubes with vacancies

The central theme of our study has been to develop and apply multiscale simulation techniques to uncover the underlying atomistic mechanisms without the limitations to the system size and time scales inherent to the fully atomistic models.



Model

Depending on the physical dimension and kinetic energy, incident accelerated ions can either penetrate the freestanding graphene or collide with the atoms of the 2D crystal to produce various vacancies for sputtering.

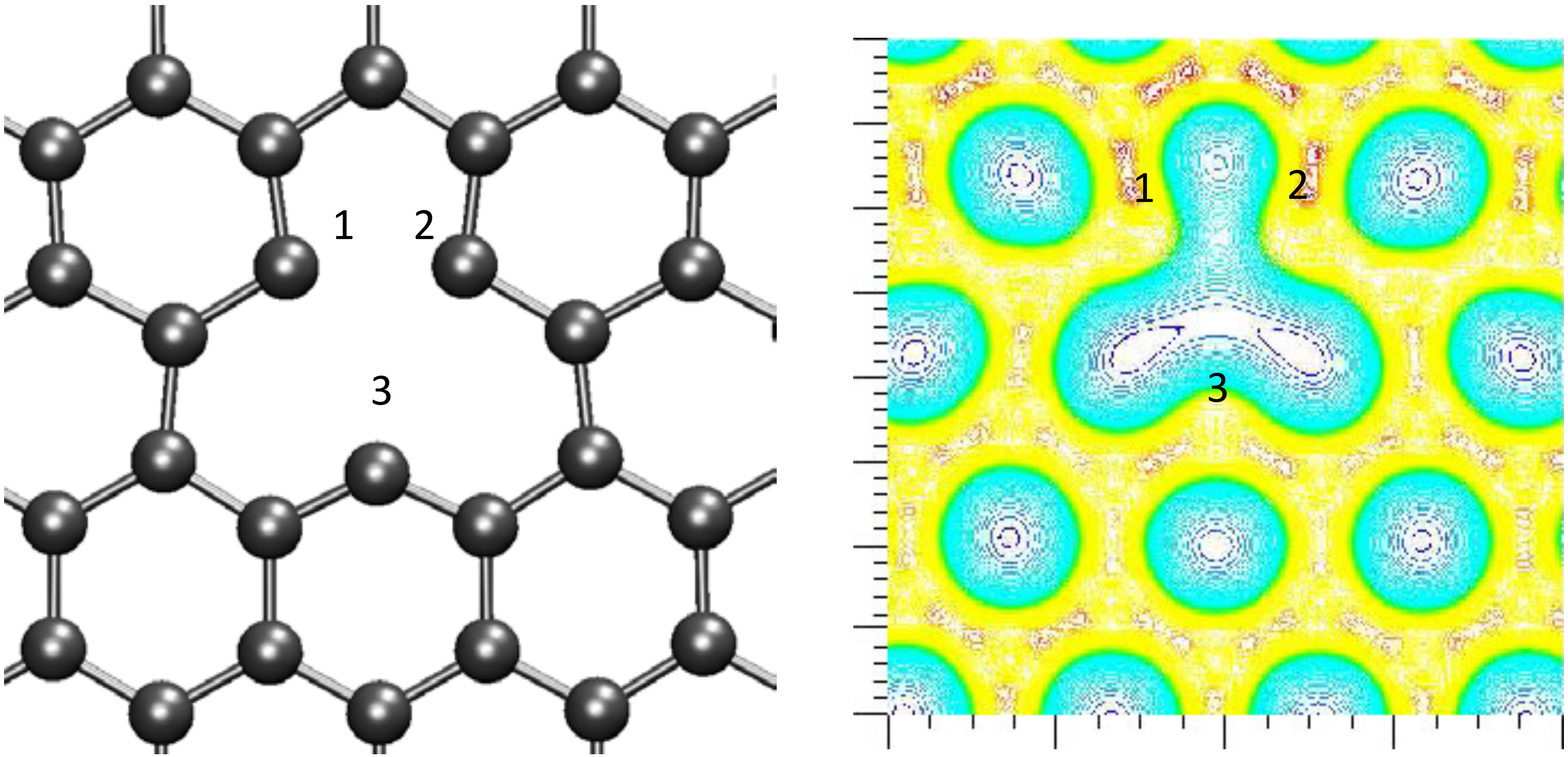
We rationalize these interactions by assuming a **binary collision process** between incident ion and the graphene lattice.

Graphene, a planar single sheet of sp2-bonded carbon atoms arranged in a honeycomb lattice

(a) Atomic structure of the vacancy in the graphene plane;

(b) charge density of the vacancy in the graphene plane (e/Å^3)

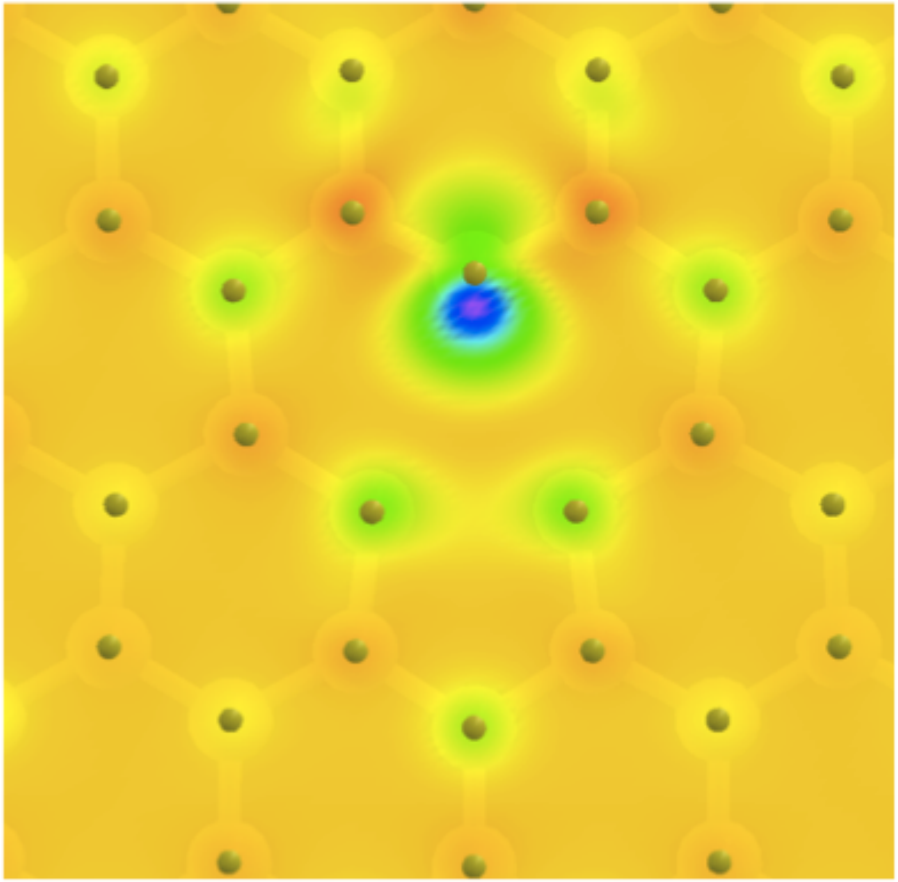
(a) 1 (b)



Results (2011 – 2016)

Introduction of vacancy defects in graphene induces magnetism, caused by quasilocalized states and dangling bonds of the surrounding atoms.

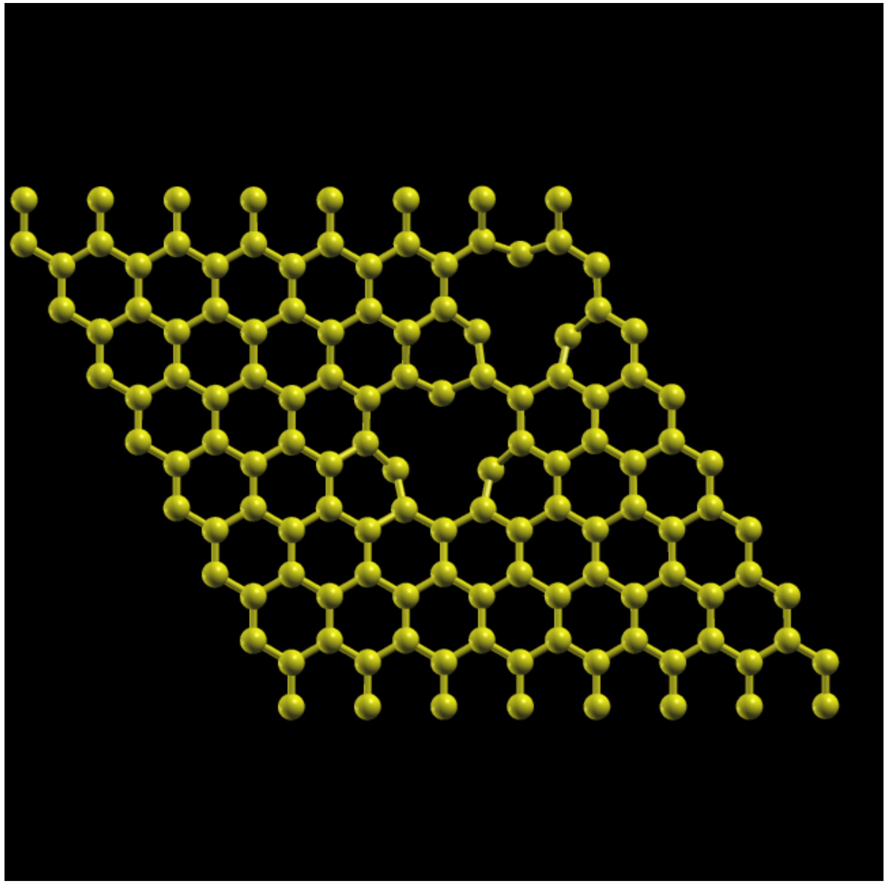
The interaction between the atoms, which occupy **the same sublattice is feromagnetic, while** . This influences the induced by the vacancy magnetization of the atoms, which is opposite for the two sublattices and decreases with increasing the distance from the defect position.



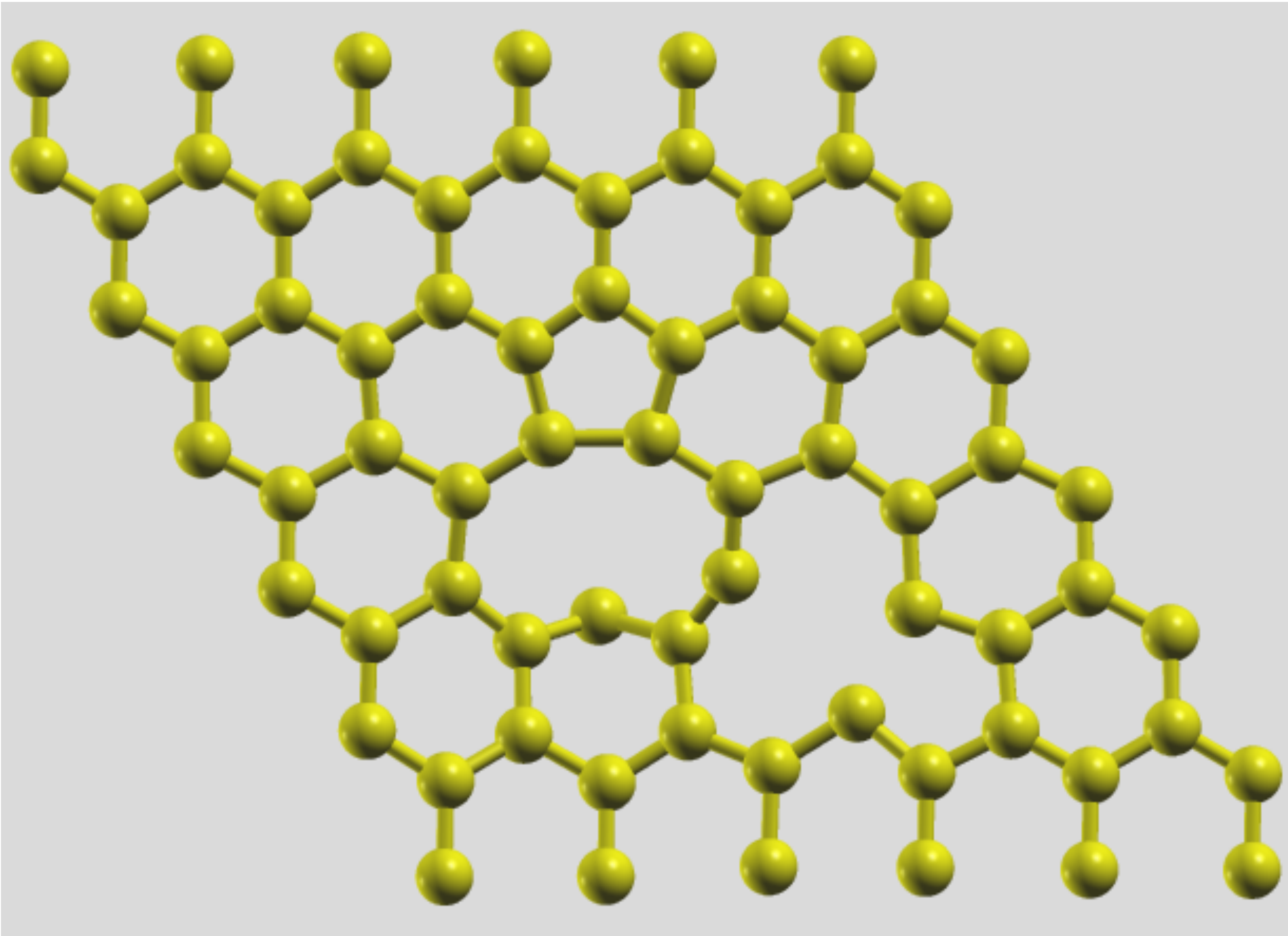
Results 2017-2018

More defects

More planes

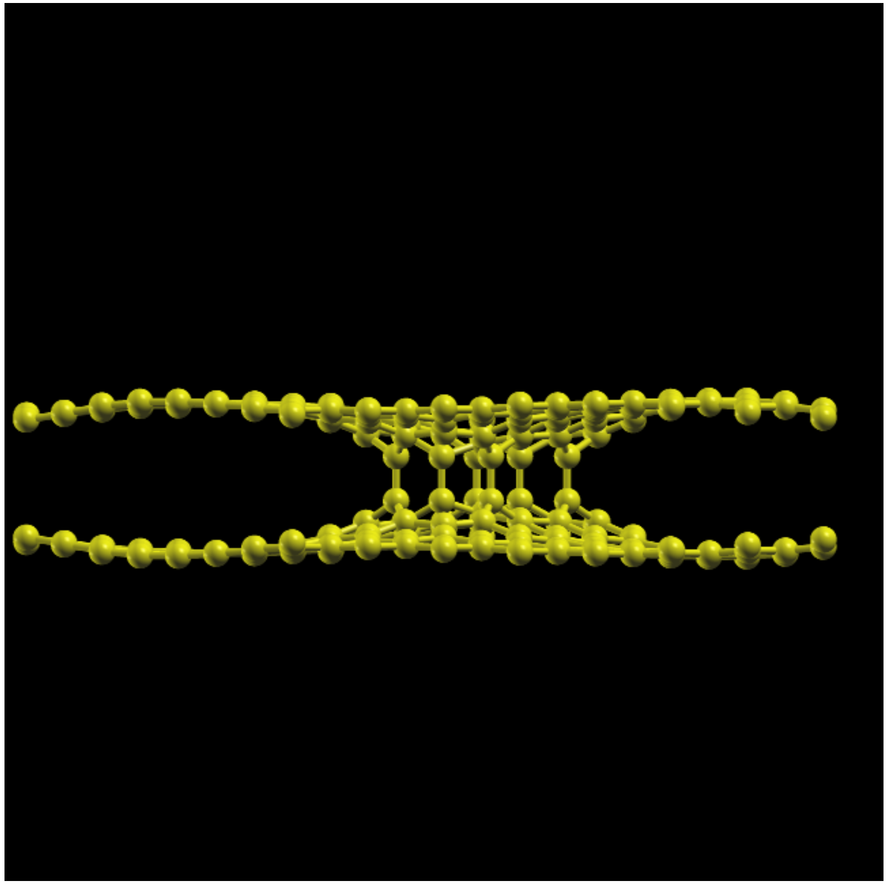


Defect relaxation

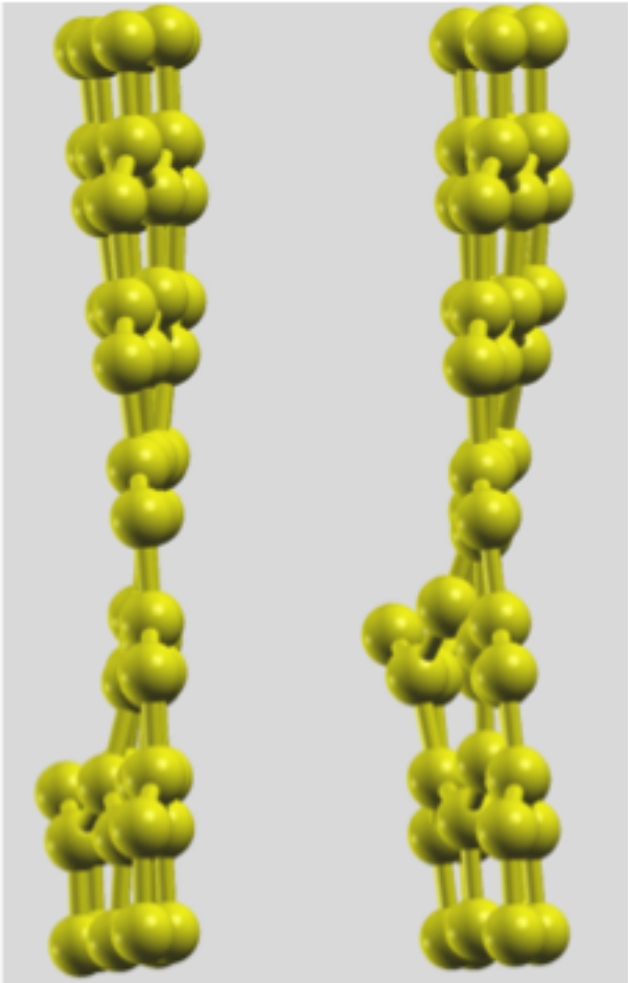


No magnetic moment generated

The bridging of graphene planes due to the defects produced by proton irradiation have been demonstrated to be the energetically favorable configuration



Vacancies in the two layers are opposite to each other (no bond)



the closest distance between the two layers is 3.44 Å

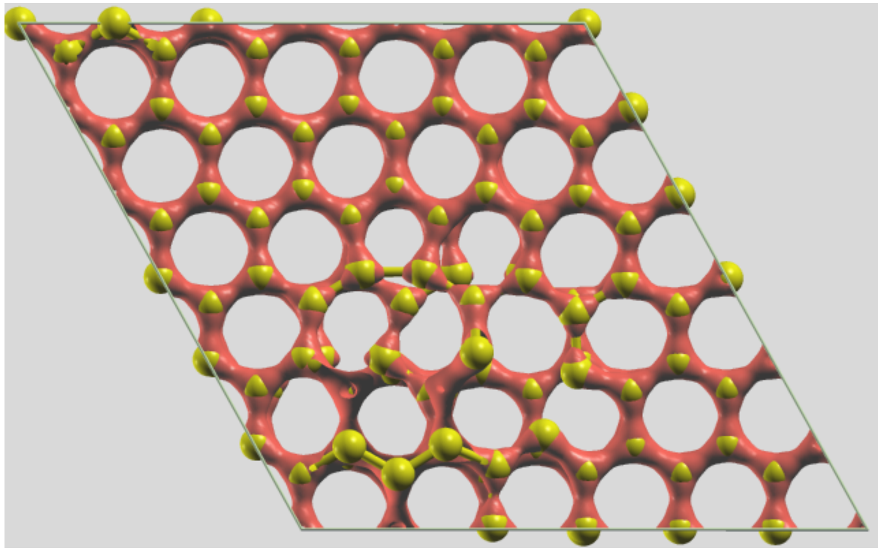
(initially the distance was set to 3.3 Å).

The longest distance (upper and lower parts) is 5.03 Å.

Final

The spin density is non-uniformly distributed among the atoms around the vacancies.

Depending on the nearest neighbors vacancies distribution, a non-zero magnetic moment of AA bilayer graphene (semiconductor) occurs.



Proton bombardment

Generates vacancies in more than one layer at the same lattices – magnetic moment

Unlike electron beam – due to scattering the probability of generating vacancies at different lattices is higher – relaxation of defects and bond formations prevent from generating a magnetic moment.

Acknowledgement

The contract D-055-2018/20.06.2018 with the Research & Development & Innovation Consortium of the Sofia Tech Park for the financial support and the computational resources of the HPC laboratory.

Thank you for your attention

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