Study resolves controversy about electron structure of defects in graphene

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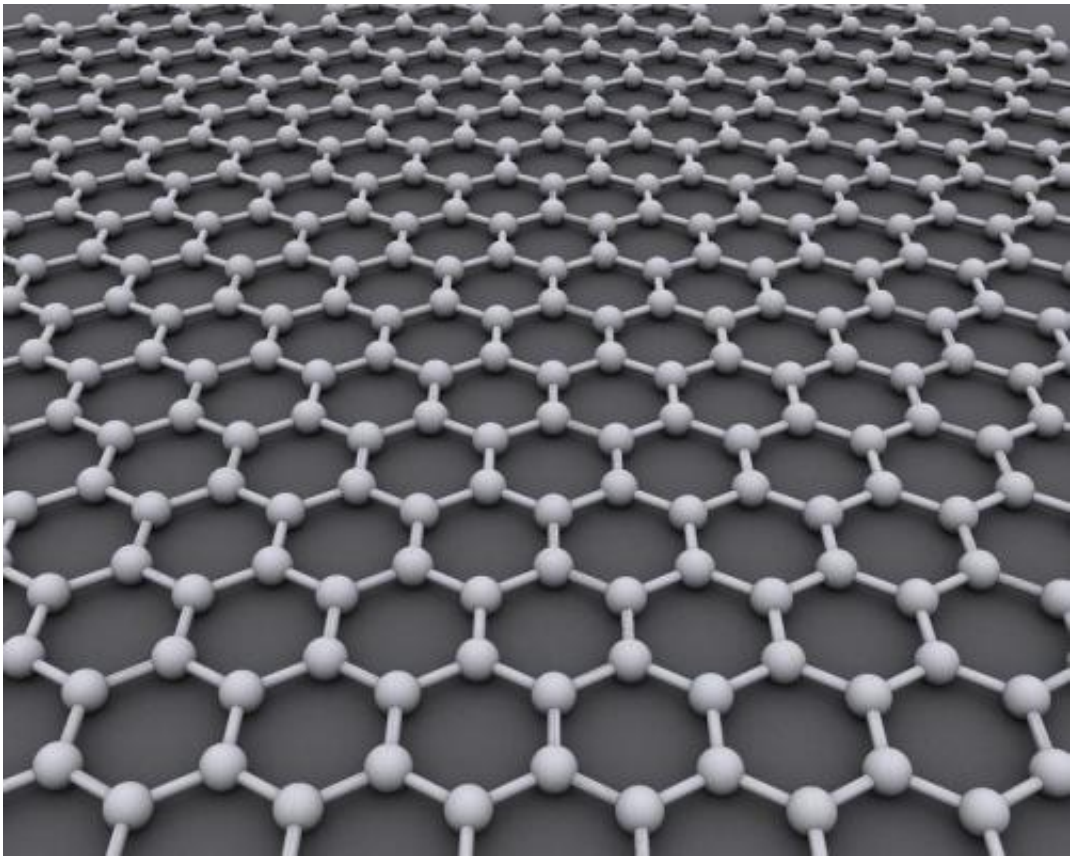

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A study conducted at the University of São Paulo's Physics Institute (IF-USP), Brazil, has resolved a longstanding controversy regarding defects in graphene. The controversy is related to the calculation of the overall electronic structure of defects. This configuration, which comprises

many variables, was described in different ways depending on the researcher and the model used. The solution, which is identical for all models and compatible with experimental findings, was obtained by Chilean Ana María Valencia García and her PhD supervisor, Marília Junqueira Caldas, Full Professor at IF-USP.

An article authored by both researchers has been published in the journal *Physical Review B*, titled "Single vacancy defect in graphene: Insights into its magnetic properties from theoretical modeling."

"There were divergences in the community regarding whether the vacancy formed by removing a single carbon atom from a graphene sheet's crystal lattice causes a weak or strong magnetic moment, and regarding the strength of the magnetic interaction between vacancies," Caldas said. The vacancy prompts the surrounding atoms to rearrange themselves into new combinations to accommodate the absence of an atom, forming electron clusters known as "floating orbitals" at the vacant site.

Three important variables are associated with the phenomenon: electron density, i.e., how the electrons are distributed; electron levels, i.e., the energy levels occupied by the electrons; and magnetic moment, i.e., the torque produced in the electrons by an external magnetic field.

First-hand use of hybrid method in graphene

"There are two ways to calculate the overall electron structure of the vacancy region, both derived from quantum mechanics: the Hartree-Fock (HF) method, and density functional theory (DFT). In DFT, the calculation is performed by making each electron interact with average electron density, which includes the electron in question. In HF, the operator used excludes the electron and considers only its interaction with the others. HF produces more precise results for electron structure

but the calculation is far more laborious," Caldas said.

"The two methods are often combined by means of hybrid functionals, which have been mentioned in the scientific literature since the end of the 20th century. I worked with them myself some time ago in a study on polymers, but they had never been used in the case of graphene. What Ana María Valencia García and I did was discover the hybrid functional that best describes the material. Applied to several models using computer simulation, our hybrid functional produced the same result for them all and this result matched the experimental data."

Besides resolving the controversy, which had lasted years, another interesting aspect of this research is the problem that motivated it. "We came to it via the interest aroused by a material known as anthropogenic dark earth or ADE," Caldas explained. "ADE is a kind of very dark, fertile soil found in several parts of the world, including the Amazon. It retains moisture even at high temperatures, and remains fertile even under heavy rain. It's called anthropogenic because its composition derives from middens and cultivation by indigenous populations in the pre-Columbian period at least two millennia ago. This intriguing material was known to have resulted from multi-stacked layers of graphene nanoflakes. It was our interest in ADE that led us to study the phenomenon of vacancy in graphene sheets."

In conclusion, it should be noted that there are potential applications of vacancy in graphene sheets, since information can be encoded in the defect and not in the entire structure. Much more research will be needed before applications can be developed, however.

More information: A. M. Valencia et al, Single vacancy defect in graphene: Insights into its magnetic properties from theoretical modeling, *Physical Review B* (2017). DOI: 10.1103/PhysRevB.96.125431

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