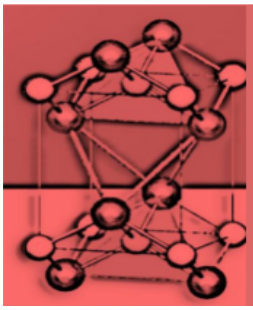

IX Workshop on Novel Methods for Electronic Structure Calculations

10th – 19th November 2021
La Plata – Argentina

Systematic Studies of Graphenic Systems in the Search of Applications

Ricardo Faccio [a], Dominique Mombrú [a], Mariano Romero [a], Alvaro Mombrú [a],
[a] *Centro NanoMat, Grupo de Física, DETEMA, Facultad de Química, Universidad de la República, Montevideo, Uruguay.*

email:

Graphene is a material with very exceptional properties which has encouraged very intense research worldwide. However, these properties should be improved through controlled modifications for the application to be feasible.
We undertook a research of graphenic materials -graphene and graphene quantum dots- where DFT simulations were carried out in systems where defects systematically distributed were included.
We used the complementary figure to implement the systematic study and to extract useful conclusions -i.e. the figure formed by the carbon atoms removed to build a vacancy. The occurrence of magnetism, distortions and rippling are features that take part of this study and that help to make useful description to guide the controlled synthesis to be carried out.
Acknowledgments: authors wish to thank PEDECIBA, CSIC-Udelar and ANII for financial support.