Editorial

The November 2023 cover paper

Maude Jimenez[1,*]
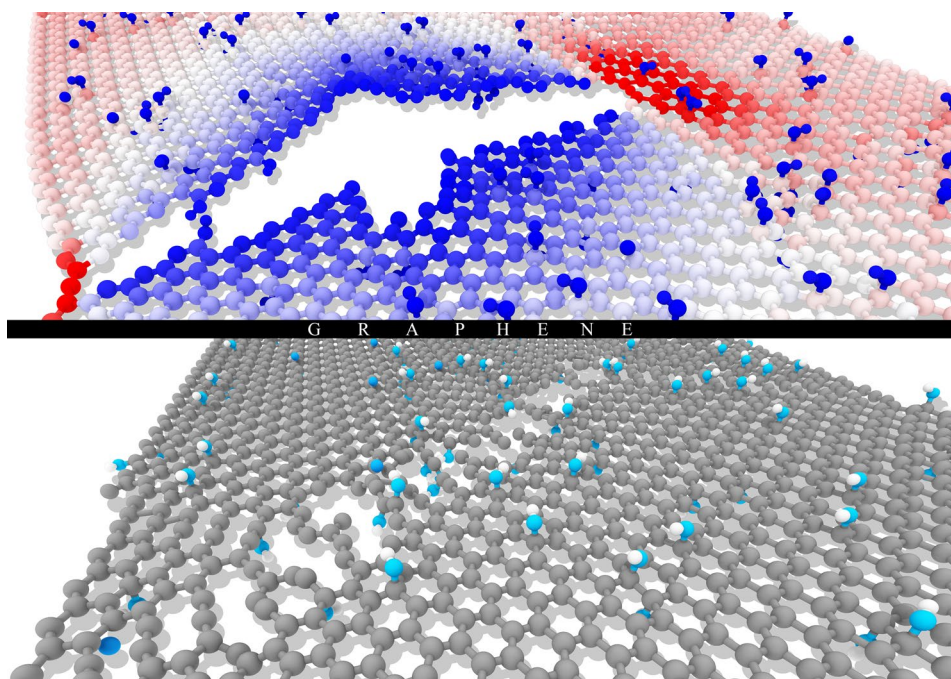
[1] *Univ. Lille, CNRS, INRAE, Centrale Lille Institut, UMR 8207, UMET - Unité Matériaux et Transformations, Lille, France*

GRAPHICAL ABSTRACT

The cover for the November 2023 issues of the Journal of Materials Science comes from the paper by Carlos Sáenz Ezquerro and his colleagues which was published in Volume 58, issue #33 from September 2023 [1]. The paper was handled by our editor Ghanshyam Pilania and is entitled "Molecular modelling of graphene nanoribbons on the effect of porosity and oxidation on the mechanical and thermal properties". It is part of our "Computation & Theory" Topical Collection. It results from a collaboration between Aragon

Address correspondence to E-mail: maude.jimenez@univ-lille.fr

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Institute of Technology ITAINNOVA and the University of Zaragoza, both based in Saragossa, in Spain.

This paper is related to graphene and graphene oxide, materials that attract worldwide attention due to their unique properties that make them highly promising materials to advance emerging technologies, from biomaterials to aerospace. Graphene nanoribbons are strips of graphene with width less than 100 nm. Their experimental characterization is usually limited to the determination of structural parameters, but the evaluation of their mechanical and thermal properties as individual nanoparticles is a challenge, touching the limits of high-resolution techniques and also often relying on technician skills.

In this paper, the authors choose to go beyond these experimental techniques by proposing nanoparticles molecular dynamics simulations. They report the development of a series of molecular-based models of graphene and graphene oxide nanoribbons with different percentages of pores, allowing to evaluate from a statistical point of view the effect of porosity and oxidation on the mechanical properties and in-plane thermal conductivity.

The authors prove in this long and detailed paper (22 printed pages, 17 figures and 103 references) the necessity to carefully consider both oxidation and porosity when tuning synthetic pathways. Molecular Dynamic simulation, using LAMMPS simulation code, is highlighted as an effective technique to compute these properties of graphene derivatives, and to obtain exploitable results that are currently difficult, if not impossible, to obtain using the most advanced experimental characterization techniques. This opens the door to future tuning of graphene properties through molecular dynamics simulations.

The researchers performing the work are shown below together with their brief bios.

Carlos Sáenz Ezquerro: Carlos Sáenz (CS) received degree in Chemistry in 2011 from University of Zaragoza. He started working at ITAINNOVA in the Division of Materials and Components in 2011. His main scientific activity has been focused on the study of polymeric nanocomposites both theoretically, through the application of Molecular Dynamics (MD) technique, and experimentally. Currently, he is finishing PhD studies in Mechanical Engineering.

Manuel Laspalas: Manuel Laspalas received PhD in Industrial Engineering from the University of Zaragoza. In 1999, he joined ITAINNOVA as a R&D engineer. His lines of research include advanced materials characterization and modelling for product performance and manufacturing processes simulation. He currently coordinates the ITAINNOVA R&D line "Sustainable Material Transformation Processes" (2021–2024)′

José Manuel García Aznar: José Manuel García-Aznar received his PhD in Mechanical Engineering in 1999 from University of Zaragoza, where he serves since 2008 as Full Professor in the Mechanical Engineering Department. In these years, he has been visiting researcher at Keele University (2001), KU Leuven (2012), Cambridge University (2015), NUI Galway (2017) and University of Oxford (2019). His research interests focus on multiscale and multiphysics computational modelling.

Susana Castelar Ariza: Susana Castelar Ariza received her PhD in Chemical Sciences in 2013 from University of Zaragoza in the group of Liquid Crystals and Polymers, focusing her research on liquid crystals dendrimers with potential applications in the fields of Materials Science and Biomedicine. In 2006, she worked at the University of Münster (Germany) studying the synthesis of molybdenum and tungsten thioderivatives, and since 2012, she works at ITAIN-NOVA in the Materials and Components Department

developing composite materials and nanomaterials for improving the final materials properties.

Agustín Chiminelli: Dr. Agustín Chiminelli Sarría received his PhD in Materials Engineering and is ITAINNOVA's researcher since 2007. His field of expertise concerns polymer matrix composite materials and adhesives. Currently, he is responsible of the R&D line about Smart and Multifunctional Materials.

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Reference

[1] Sáenz Ezquerro C, Laspalas M, García Aznar JM et al (2023) Molecular modelling of graphene nanoribbons on the effect of porosity and oxidation on the mechanical and thermal properties. J Mater Sci 58:13295–13316. https://doi.org/10.1007/s10853-023-08810-y