

Properties and Applications of Grazynes: Carbon-Based 2D Composites

Pablo Gamallo

Adrià Calzada, Francesc Viñes

Departament de Ciència de Materials i Química Física & Institut de Química Teòrica i Computacional (IQTCUB), Universitat de Barcelona, C. Martí i Franquès 1, 08028 Barcelona, Spain
gamallo@ub.edu

Abstract

Our research group has put forward a novel group of two-dimensional carbon structures derived from graphene, where graphene strips are interconnected through acetylenic bonds. Due to the diverse connectivity options available, we have categorized these structures into a new family termed "grazynes" [1]. In our investigation, we focused on DFT derived energetic, structural, elastic and electronic properties of simplest grazynic configurations as [1],[1]{0}-grazyne, [2],[1]{0}-grazyne, and [3],[1]{0}-grazyne.

Our findings reveal that grazynes represent intriguing yet stable materials, exhibiting greater stiffness than graphene along the acetylenic direction. They display significant anisotropy and feature Dirac points in reciprocal space along the direction of graphene strips, showing remarkable resistance to strain regardless of its orientation. Consequently, grazynes demonstrate directional electron conductivity facilitated by acetylene-mediated electron transport and exhibit resilience to stretching/compression, which is crucial for potential applications in nanoelectronics [2].

Furthermore, certain grazynic structures may possess defects or porosity, making them promising candidates for applications in gas separation. This is the case of [1],[1,2]{0,1}-grazyne, [1],[2]{2}-grazyne, and [1],[2]{(00),2}-grazyne shown in Figure 1. To explore the potentiality of these structures for acting as molecular sieve, we conducted molecular dynamics simulations to evaluate the performance of grazynic membranes for tasks such as biogas upgrading and various gas separation processes [3].

References

- [1] S. Kamalinahad, F. Viñes, P. Gamallo, *J. Phys. Chem. C*, 123 (2019) 2714.
- [2] I. Alcón, N. Papior, G. Calogero, F. Viñes, P. Gamallo, M. Brandbyge, *J. Phys. Chem. Lett.*, 12 (2021) 11220.
- [3] F. Viñes, A. Calzada, P. Gamallo, *J. CO2 Util.*, 71 (2023) 102459.

Figures

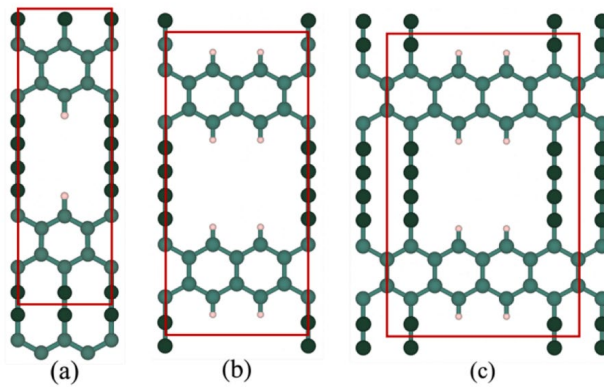


Figure 1: Insert caption to place caption below figure (Century Gothic 10) Top view of (a) [1],[1,2]{0,1}-grazyne, (b) [1],[2]{2}-grazyne, and (c) [1],[2]{(00),2}-grazyne (white: H atoms, dark green: sp C atoms, light green: sp² C atoms).