DFT study of nanoporous graphene filled by heteroatoms as catalysts

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Graphene exhibits a low chemical reactivity that limits its electrocatalytic applications. But, according to the reports published, the substitution of C atoms in graphene's lattice with B and N atoms is an efficient way to enhance its chemical reaction [1][2]. However, a step further in the efficiency could be achieved by controlling the distribution of the dopants all along the membrane.

In this work, we propose to use the nanoporous graphene (NPG) obtained by Moreno et al. [3] as a template to obtain a heteroatom-doped graphene membrane with equal active sites that are evenly distributed in the lattice. For that, we propose to fill the regular pores of the atomically precise 2D carbon-based material with triazine and borazine molecules.

By employing Density Functional Theory (DFT) the resulting heteroatom doped graphene-based membranes have been characterized by analyzing their electronic properties. Furthermore, to test how the chemical reactivity of these dopants improves graphene's reactivity, we have also investigated the CO_2 reduction reaction (CO_2RR) catalyzed by these materials. Our results for CO_2RR pave the way to explore other interesting reactions, e.g., the oxygen evolution reaction (OER).

References

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[3] Moreno, C., Vilas-Varela, M., Kretz, B., Garcia-Lekue, A., Costache, M., & Paradinas, M., Panighel, M., Ceballos, G., Valenzuela, S.O.,Peña,D., Mugarza, A., Science, 360(2018) 199-203

Figures

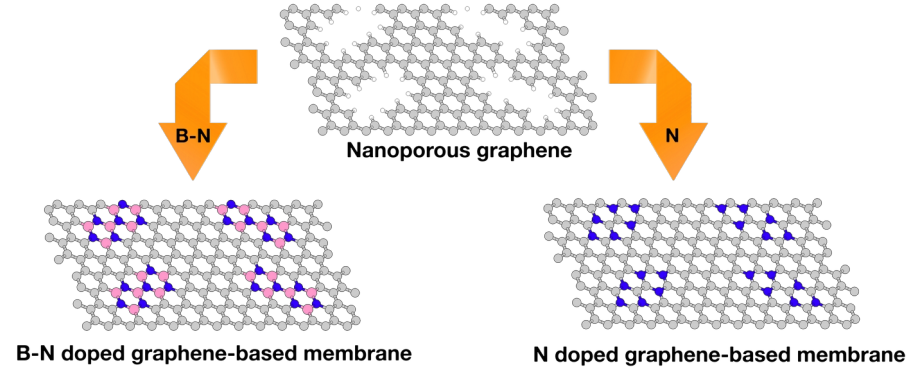

Figure 1: Filling of the pores in NPG to obtain heteroatom-doped based membranes.