Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


# Supplementary Material

# ADSORPTION OF ANTI-INFLAMMATORY NIMESULIDE BY GRAPHENE MATERIALS: A COMBINED THEORETICAL AND EXPERIMENTAL STUDY

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The Fig. S1. show the structural and electronic properties of NM drug.

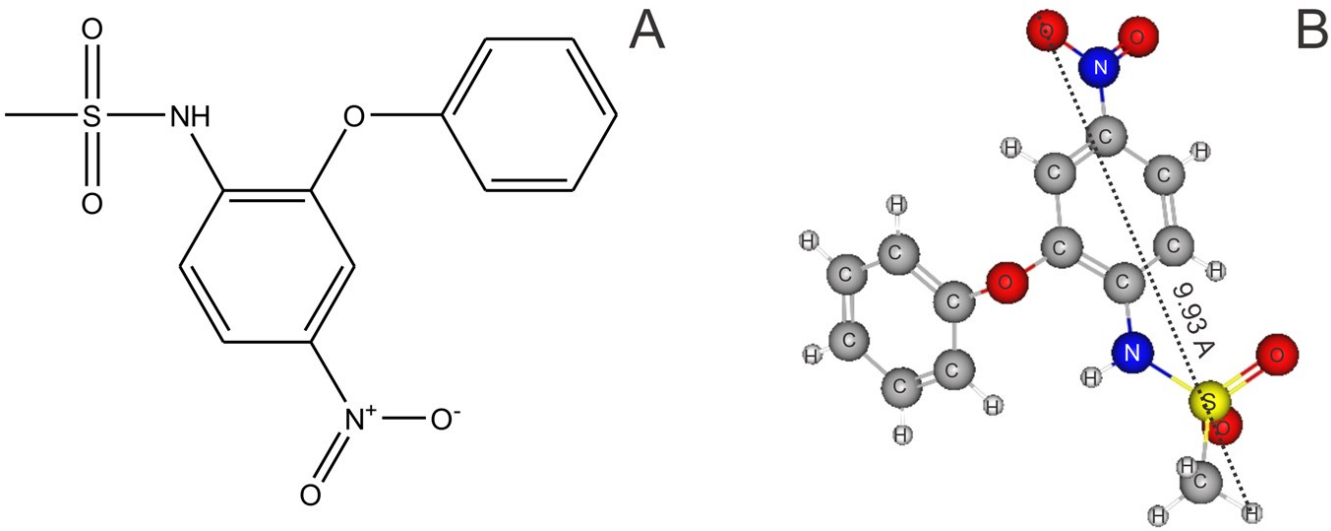


**Fig. S1** (A) Structural formula of NM; (B) Optimized three-dimensional structural formula of NM. The dimensions of the chemical molecule was calculated using MarvinSketch version 17.3.27. Van der Waals surface area = 406.45 $A^2$ (pH 7.0-14.0); Polar surface area 104.12 $A^2$ (pH 7.0-14.0); Van der Waals volume = 249.10 $A^3$; Dipole Moment 11.75 Debye; Log P 1.79, Davies HLB (Hydrophylic-lipophilic balance) = 5.02.

The Fig. S2A display the optimized molecular structure of graphene exposes a planar geometric configuration throughout its entire length, being C-C distance about 1.42 Å. The conduction and valence bands meet at the K point of the Brillouin zone.

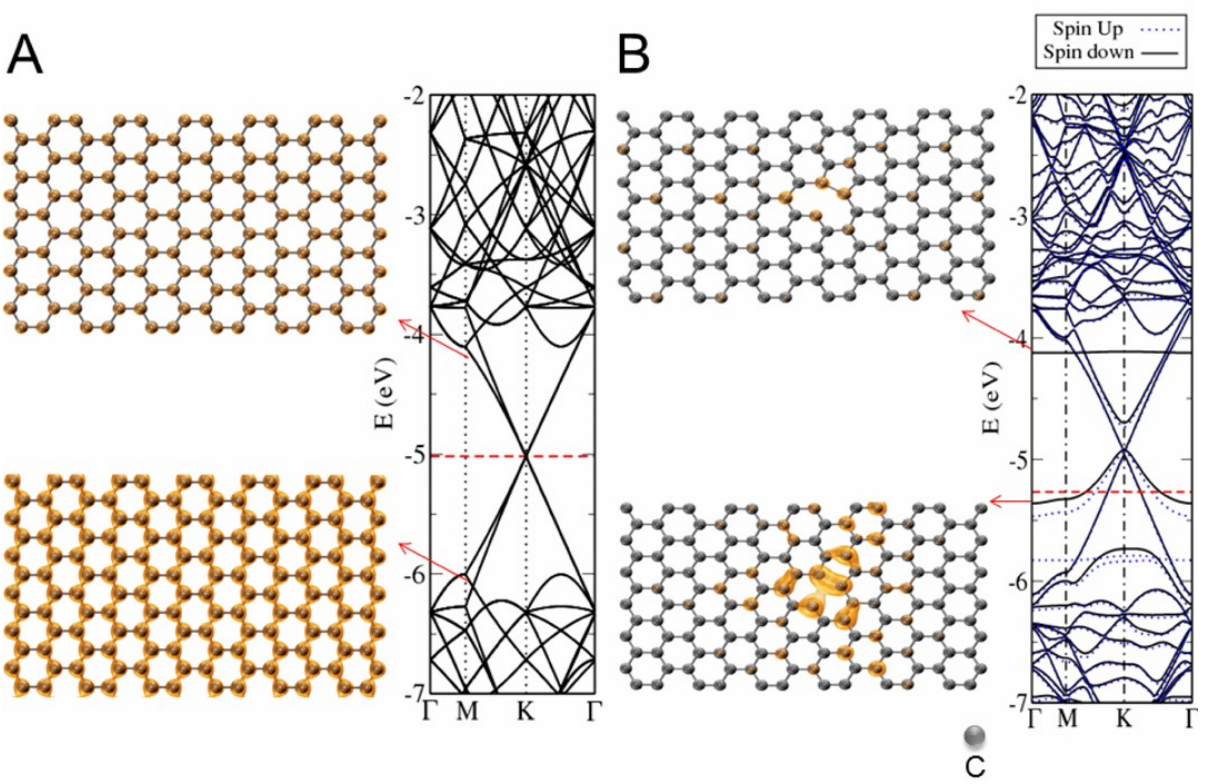


**Fig. S2** Optimized structure, density of charges and band structure to (A) pristine graphene, (B) graphene plus a vacancy.

Generating a vacancy on grapheme plane by removing a carbon atom, leads to an alteration on the surface of graphene and repositioning of atoms, originating a pentagon on hexagonal structure of graphene plane. Thus, the bond distance between two neighboring atoms in pentagon varies to 1.76 Å. Furthermore, there is a small displacement (~0.1 Å) out of the basal plane of graphene, from the atom on the

opposite side of former pentagon (Fig. S2B). All these distortions takes a hybridization levels and a spin polarization about 1.16 μB in graphene.

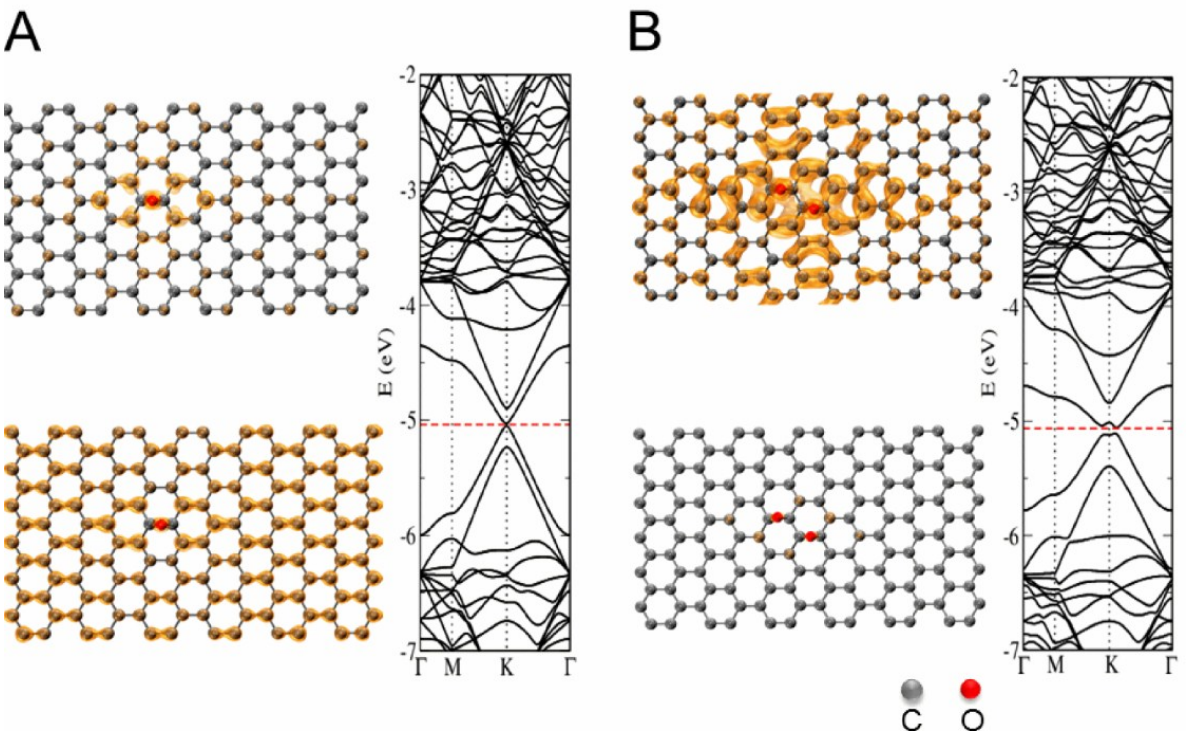


**Fig. S3** Optimized structure, density of charges and band structure to (A) graphene + 1 epoxy group, (B) graphene + 2 epoxy groups.

For epoxy functionalized graphene, the functional groups exhibit a displacement out of graphene plane, being more significant to graphene with two epoxy groups (about 0,45 Å). The C-O distance, was around 1.44 Å while the C-C distance, near functional groups, increased to 1.51 Å for one other two epoxy groups (Fig. S3A and S3B). Breaking on symmetry, degeneration levels and also a gap opening on graphene (more visible to graphene with 2 epoxy).

To graphene functionalized with one or two hydroxyl groups, once again where found a displacement of carbon atoms out of basal graphene plane around 0.44 Å to one hydroxyl group, and 0.53 Å for two hydroxyl groups. The C-C distance on hydroxyl groups was approximately 1.51 Å, while C-O and O-H distances stay around 1.48 Å and 0.98 Å respectively (Fig. S4A and S4B). The atomic distortions of graphene plane lead to a separation of some degenerate levels. The presence on band structure of a flat level between the valence and conduction band, as well as an opening of a small gap (~ 0,1 eV). Degenerate levels and a gap opening (~0.2 eV) become even more evident to graphene functionalized with two hydroxyl groups.

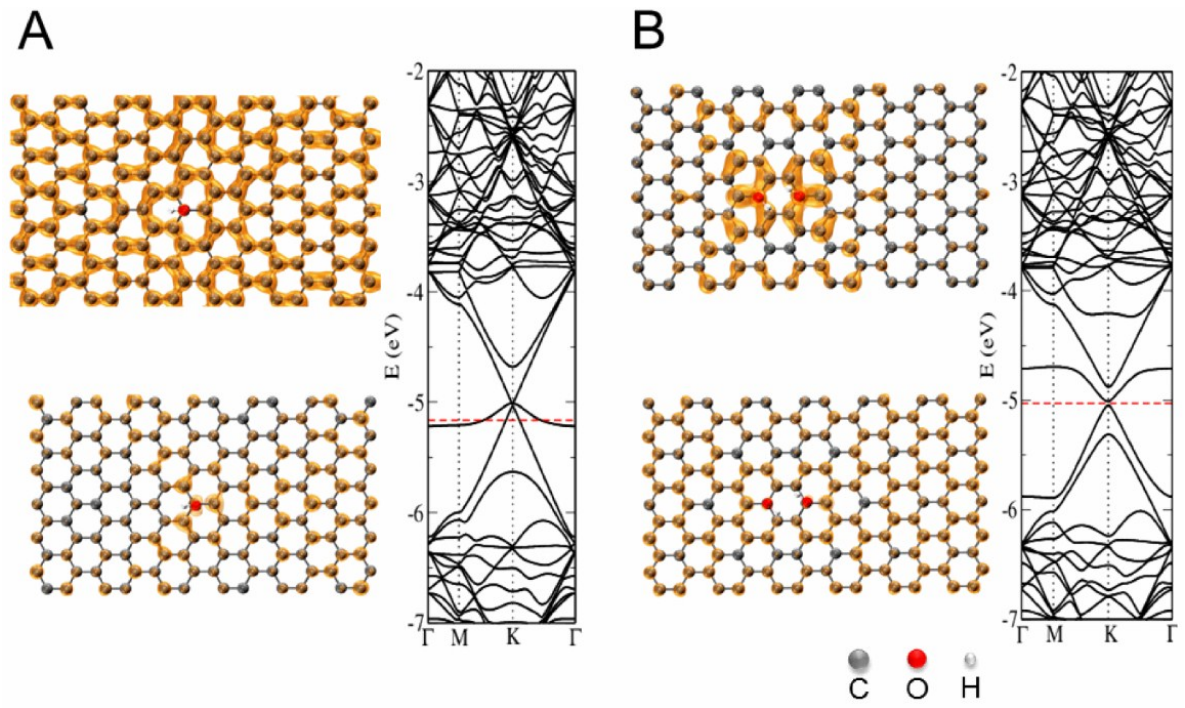


**Fig. S4** Optimized structure, density of charges and band structure to (A) graphene + 1 hidroxyl group, (B) graphene + 2 hydroxyl groups.

Regarding as graphene nanoribbons functionalized with one or two carboxyl groups respectively (Fig. S5A and S5B), it was founded that carbon atoms of hydroxyl groups present a displacement out of nanoribbon plane around 1.35 Å and 1.44 Å to one and two functional groups, respectively. Furthermore, to one carboxyl group the angle between $O_1$-$O_2$ was 121.88°, while the angle $O_2$-H was 103.94°. The distances between C-C, $O_1$-$O_2$ and $O_2$-H, were around 1.22 Å; 1.35 Å and 0.99 Å, respectively. For two carboxyl groups the angle between $O_1$-$O_2$ was 120.9°, while the $O_2$-H angle was 105°. The distances between C-C; $O_2$-$O_1$ and $O_2$-H, were similar to the previous ones, i.e. around 1.22 Å; 1.35 Å and 0.99 Å, respectively (Fig. S5A and S5B).

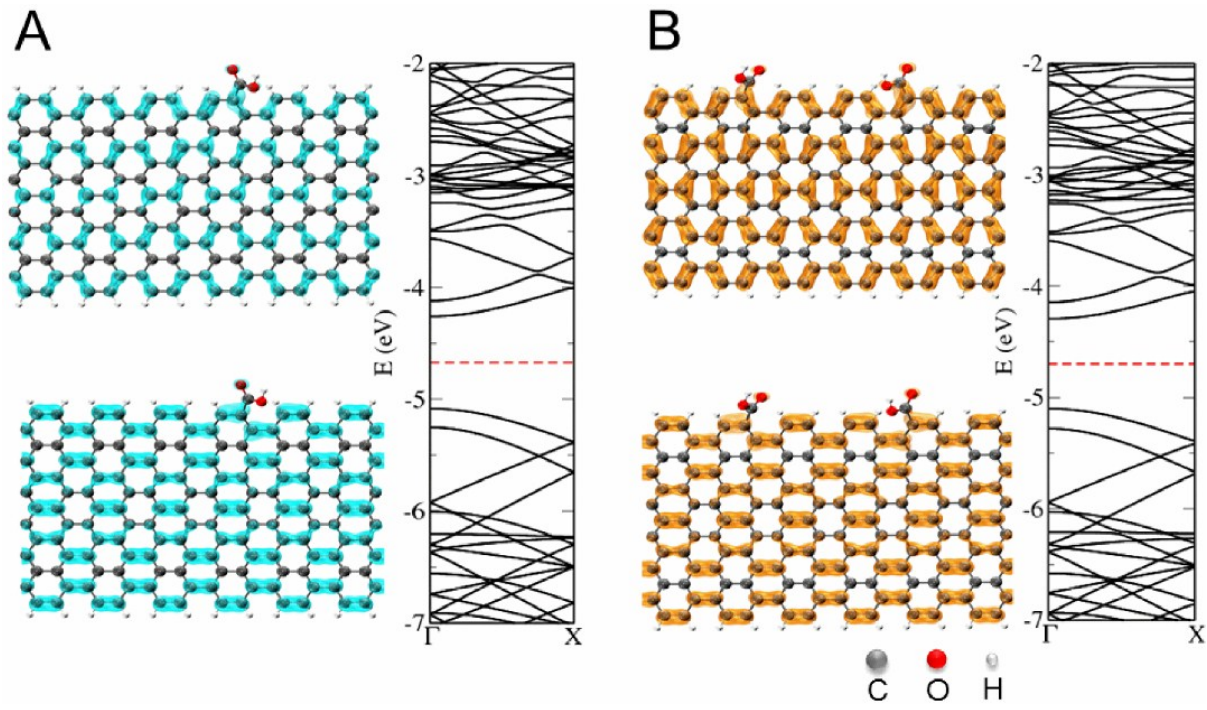


**Fig. S5** Optimized structure, density of charges and band structure to (A) graphene nanoribbon + 1 carboxyl group, and (B) graphene nanoribbon + 2 carboxyl groups.

To configurations evolving graphene nanoribbons functionalized with one or two carbonyl groups, respectively (Fig. S6A and S6B), it was founded that functional groups remained at the same height in relation to nanoribbon plane, unlike to carboxyl group. Furthermore, for both, nanorribon with one or two carbonyl groups, C-O distances were approximately 1.25 Å, whereas the distances between neighboring carbon of carboxyl group are in the range of 1.43 Å to 1.47 Å. Also can be notice the presence of flat levels on the Fermi level (see Fig. S6A and S6B). This can be attribute to C-O functional group, where in these cases shows absence of 1 electron. Thus, there is a strong trend of this functional group to receiving one electron.

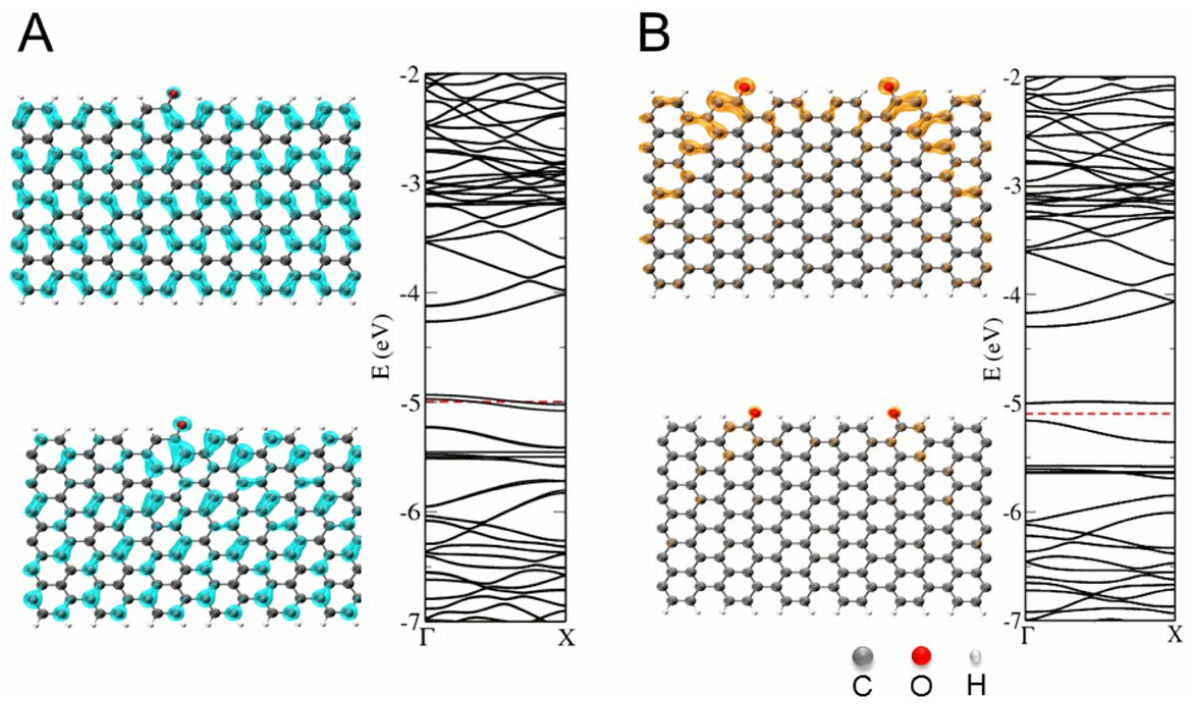


**Fig. S6** Optimized structure, density of charges and band structure to (A) graphene nanoribbon + 1 carbonyl group, (B) graphene nanoribbon + 2 carbonyl groups.

The Fig. S7 display a photograph of the NM solution before and after the

adsorption process by rGO.

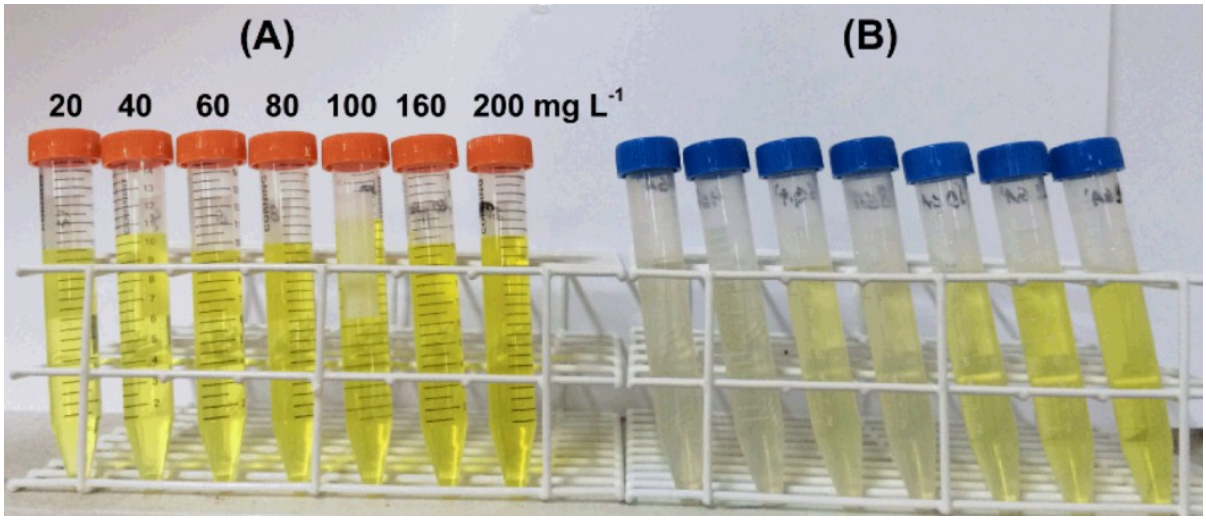


**Fig. S7** Photograph of the NM solutions (20.0 to 200.0 mg $L^{-1}$) (A) before and (B) after, respectively, of the adsorption process by rGO.