In the crib: how Graphyne cradles the natural amino acids

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Graphene is widely heralded for extensive applications in distinct, but converging, areas that include nano and regenerative medicine, anticancer/antibacterial approaches, and drug delivery. It can also be the active material for bioimaging, biosensing and photo-therapies (both photodynamic, PDT, and photothermic, PTT).

Graphane is its hydrogen-saturated counterpart, graphyne its acetylene-based 2D analogue. Both of these carbon allotropes are endowed with physico-chemical properties that in some cases improve those of graphene. In biomedicine, graphane and graphyne have generated interest for biosensing and for PTT anticancer therapy. Much of the theranostic potential of these 2D materials relies on their ability to interact with biological targets, which are largely proteins and peptides. [1,2]

A deep knowledge of the interaction underlying the affinity of graphane, graphene and graphyne for proteins is therefore crucial for their nanotechnological and nanomedical applicability.

Here, we investigated the atomistic details of the interaction between amino acids and graphane, graphene, and graphyne. We determined the binding energies of all twenty natural amino acids for these materials by means of Molecular Dynamics (MD) simulations and Molecular Mechanics/Generalized Born Surface Area (MM-GBSA) method.

Aromatic amino acids, such as tryptophan, phenylalanine, and tyrosine, but also arginine with its guanidinium group, show the highest affinity for graphane, graphene and graphyne (Figure 1). This trend is readily understood on the basis of $\pi - \pi$ interactions, which drive the binding.

The "corrugated" surface of graphane displays the lowest affinity towards the amino acids because of the presence of protons that shove the amino acid away from the carbonaceous basal plane. Graphyne has the highest affinity for the amino acids. This 2D material is able to cradle the amino acid increasing the number of interactions.

References

[1] A. Ferrari, F. Bonaccorso, et al. *Nanoscale*, 2015, 11, 4598-4810 .
[2] M. Pumera, C. H. A. Wong, *Chem. Soc. Rev.* **2013**, *42*, 5987-5995.

Figures

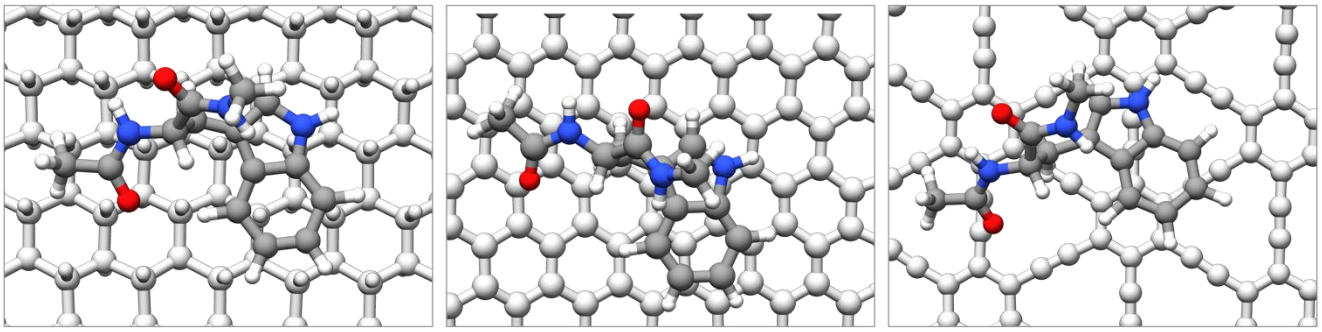

Figure 1: Representation of the interaction of tryptophan with graphane (left panel), graphene (central panel) and graphyne (right panel).