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2D host–guest supramolecular chemistry for an on-monolayer graphene emitting platform

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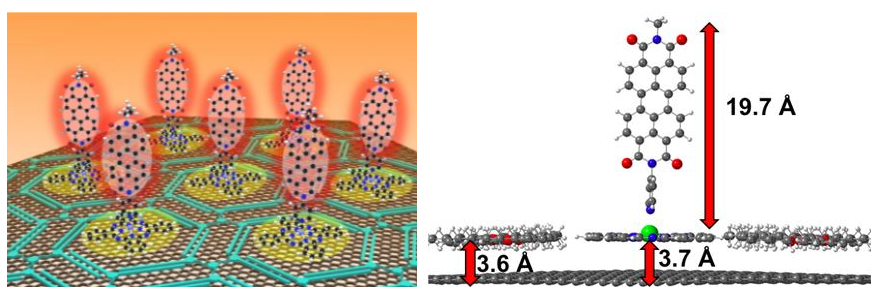
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Abstract:

Electronic decoupling of molecular chromophores from graphene to preserve their optical properties with the objective to elaborate light-responsive hybrid system for new electronic and optoelectronic nanodevices remains largely unexplored.¹

Here, we demonstrate for the first time an easy-to-implement strategy that successfully tackles the electronic decoupling issue.² Graphene-confined supramolecular host-guest recognition is used to elaborate an emitting hybrid platform. This noncovalent functionalization approach, based on two-dimensional (2D) host-guest supramolecular chemistry, enables immobilization of emitting 3D guest molecules into a 2D self-assembled porous template. It is shown that the cavities of an on-monolayer graphene nanoporous self-assembled network are able to trap zinc phthalocyanine (ZnPc) molecules coordinated to an appropriately designed emitting axial ligand (pyridine-functionalized perylene tetracarboxydiimide (Py-PTCDI)). As a result, the well-controlled graphene-chromophore and interchromophore distances combined with the mastered chromophore orientation perpendicular to the substrate, allow the elaboration of an emitting graphene-based hybrid system with the same features as the single molecular emitter, demonstrating the preservation of its intrinsic electronic properties. Furthermore, an in-depth modelling study confirms the weak interaction between the out of plane emitting moieties and the monolayer graphene.

Therefore, contrary to current photo-active graphene systems that take advantage of the direct electronic interaction (quenching) between the photo-responsive moieties and the graphene, our decoupling strategy that retains the molecular electronic properties is promising to create on demand innovative light-responsive graphene-based devices in nanophotonics and optoelectronics.



Sketched and side view of the modelled system made of a graphene layer, covered with ZnPc:Py-PTCDI emitting guest molecules trapped in the supramolecular self-assembled nanoporous host network.

References:

1. L. Sosa-Vargas, E. Kim, A.-J. Attias, *Materials Horizons* **2017**, 4, 570-583.
2. B. Kim, C. Cho, I. Arfaoui, C. Paris, C. Petit, T. Le Bahers, E. Kim, A.-J. Attias, *Materials Horizons* **2020**, 7, 2741-2748.