Novel covalent functionalization of graphene with porphyrin.

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Résumé

The chemical functionalization of graphene is critical for incorporating the carbon layer into a variety of applications including electronic devices and sensors[1].

We investigate two possible chemical reactions between iron porphyrin and a metal supported graphene. On the one hand, covalent modification of graphene via Diels-Alder reactions is emerging as a key tool to achieve this goal. Usually, graphene functions as both C4 and C2 unit when paired with a Diels-Alder partner[2]. In our case, we take advantage of the peculiar interaction between the metal and graphene in some specific areas of the moiré pattern, where a C3 fragment of graphene can present a similar electronic structure as an allyl fragment[3]. Our proposed mechanism fulfills the Woodward-Hoffmann rules and establishes a novel reversible covalent functionalization of graphene which is controlled by the underlying metal substrate[4].

On the other hand, we propose a covalent bond formation with graphene by means of dehydrogenation of one or more pyrrole groups of the porphyrin. We find that the strength of the interaction between the metal and the graphene plays a crucial role in the experimental feasibility of the reaction.

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