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Abstract title: Deterministic organic functionalization of exfoliated monolayer graphene via high-resolution surface engineering

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Abstract

Since its discovery in 2004 by Novoselov and Geim [1], graphene has triggered extensive investigation as an ideal 2D material, due to its outstanding properties. Notwithstanding the huge application potential of graphene, surface chemical functionalization would allow the possibility to finely tune the system's physical and chemical properties, amplifying the individual features of each component [2]. Spatially resolved organic functionalization of monolayer graphene with 1,3-dipolar cycloaddition of azomethine ylide, chosen because of its interest in different applications, such as pillars and sensors [3-4], is successfully achieved using low-energy electron beam irradiation, leading to a controlled local enhancing of the chemical reactivity and an original design of the functionalized area [5]. Therefore, thanks to the high-spatially resolved generation of structural defects (~100 nm), a chemical reactivity pattern has been designed over the graphene surface in a finely controlled way. The spatial distribution of the defects is investigated with AFM while Raman spectroscopy reveals new features that arise from the 1,3-dipolar cycloaddition, confirming the spatial selectivity of the graphene functionalization achieved via defect engineering. Moreover, we have investigated the Raman signature of the functionalized graphene via ab initio molecular dynamics simulations, computing the power spectrum. A further and interesting feature of 1,3-dipolar cycloaddition is its reversibility thanks to the desorption of the azomethine ylide induced by low power laser irradiation. The selective and reversible functionalization of high-quality graphene using 1,3-dipolar cycloaddition represents therefore a pivotal step for the design and realization of highly complex graphene-based devices and sensors at the nanoscale. [1] K.S. Novoselov et al., Science, 2004, **306**, 666-669.[2] A. Criado et al., Angew. Chem. Int. Ed., 2015, **54**, 10734-13750.[3] V. Georgakilas et al., Chem. Comm., 2010, **46**, 1766-1768.[4] M. Quintana et al., ACS Nano, 2010, **4**, 3527-3533.[5] L. Basta et al., J. Mater. Chem. C, 2023, **11**, 2630.