Charge Transport in Multilayer Graphene Oxide: Bulk Diffusion versus Device Properties

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Charge transport in multi-layered van der Waals materials has become an attractive and challenging problem, in the perspective of both fundamental and applied research on these structures. [1-2] We report a theoretical study of the effect on interlayer interaction in charge transport for chemically disordered graphene multilayer compounds. Using molecular dynamics and tight-binding Hamiltonian, layered disordered graphene sheets containing random distribution of epoxide and hydroxyl defects as well as divacancies and Stone-Wales type defects are modelled and their bulk and device transport properties are analysed. Bulk transport is found to become damaged by increasing the number of layers. In sharp contrast, when computing quantum transport using a device geometry and including contact effects, a different scenario is obtained, supporting the positive contribution of layer-layer interaction in increasing the effective sp^2 spatial area and favouring enhanced delocalization of electronic states. This sheds some new light on recent experimental features. [3]

Acknowledgements. We acknowledge support from the Flag-Era JTC 2017 project 'MECHANIC'. MNÇ and HS acknowledge support from TÜBİTAK (117F480). AA and SR are supported by MECHANIC reference number: PCI2018-093120 funded by Ministerio de Ciencia, Innovaci\'on y Universidades and the European Union Horizon 2020 research and innovation programme under Grant Agreement No. 881603 (Graphene Flagship). ICN2 is funded by the CERCA Programme/Generalitat de Catalunya, and is supported by the Severo Ochoa program from Spanish MINECO (Grant No. SEV-2017-0706). VHN and JCC acknowledge financial support from UC Louvain and the FNRS of Belgium.

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FIGURES