

#022 - Morphing graphene for energy applications

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In spite of its exceptional properties, for many applications bare graphene is not optimal. Its null density of states at the Fermi level limits the exploitation of its conducting properties [1]; it is weakly interacting, which limits its potentialities as medium for gas storage in spite of its exceptional surface to mass ratio. In addition, storage applications requires building 3D graphene based frameworks [2]. Therefore morphing and functionalization of graphene in controlled way are the current challenges in the field of graphene-based technologies.

Here, combined simulation-experimental studies on the relationship between graphene morphology and its electronic and chemical properties are reported. Structural deformation and rippling, defects (structural or substitutional), chemical decoration and functionalization are evaluated and the relationships between each other are shown. For instance, the presence of defects or corrugation enhances reactivity, which in turn favors the chemical functionalization [3-5]. On one side, this can directly favor both chemical adhesion and physical interaction of hydrogen with graphene[3,6-9]. On the other hand, it allows controlling the concentration and location of spacer molecules for designing of 3D pillared multilayers structures[10,11]. These studies additionally returned side-results on the relationship between structural and electronic properties, exploitable for graphene based-nanoelectronics [3,10].

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- [1] V Tozzini, V Pellegrini JPCC, **115** 25523 (2011)
- [2] V Tozzini, V Pellegrini Phys Chem Chem Phys, **15** 80 (2013)
- [3] T Mashoff, V Tozzini, et al APL **106** 083901 (2015)
- [4] S Goler, V Tozzini, et. al. JPCC **117** 11506 (2013)
- [5] A Rossi, S Piccinin, V Pellegrini, S de Gironcoli, V Tozzini JPCC **119** 7900 (2015)
- [6] K Kakhiani, V Tozzini, in preparation.
- [7] V D Camiola, T Cavallucci, A Rossi, V Pellegrini, V Tozzini FM, **2** 00003 (2015)
- [8] V D Camiola, R Farchioni, V Pellegrini, V Tozzini 2DM **2** 014009 (2015)
- [9] T Cavallucci, V Tozzini, JPC C **120**, 7670 (2016)
- [10] T Cavallucci, , MsD Thesis, Supervisor: V Tozzini (2014)
- [11] Y Murata, et al APL **105** (2015), 221604

#023 - Self-assembly synthesis of layered, vertically aligned 2D molybdenum trioxide functional scaffolds for host-guest photo-electrochemistry in hybrid organic/inorganic hydrogen evolution devices.

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