Consiglio Nazionale delle Ricerche
Istituto di Chimica dei Composti OrganoMetallici

Lunedì 25 Febbraio 2019
alle ore 11.00

presso AULA 2 dell'Edificio F
Area della Ricerca CNR
Via Madonna del Piano, 10 Sesto Fiorentino (Firenze)

il Prof. Xin Liu
Dalian University of Technology
China

terrà il seguente seminario:

Surface diffusion regulated growth of vacancy clusters on graphene oxide: a first-principles investigation

Dr. Andrea Ienco
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Biographic sketch:

- 2014-12/Now, Associate Professor, School of Chemistry, Dalian University of Technology, China.
- 2017-12/2018-12, Research Consultant, KAUST Catalysis Center, King Abdullah University of Science and Technology, Kingdom of Saudi Arabia.
- 2017-01/2017-02, Visiting Professor, Laboratoire Modélisation et Simulation Multi Echelle, Université Paris-Est, France.
- 2015-07/2015-09, Research Consultant, KAUST Advanced Membranes and Porous Materials Center, King Abdullah University of Science and Technology, KSA.
- 2006-11/2014-12, Lecturer, School of Chemistry, Dalian University of Technology, China.
- 2010-09/2012-09, Post-doc fellow, KAUST Advanced Membranes and Porous Materials Center, King Abdullah University of Science and Technology, KSA.
- 2010-02/2010-07, Visiting Scholar, Department of Physics, Rensselaer Polytechnic Institute, Troy, NY, USA.
- 2006-2/2008-12, Visiting Scholar, State Key Laboratory of Catalysis, Dalian Institute of Chemical Physics, Chinese Academy of Science, China.
- 1999-07/2000-07, Software Engineer, Dalian Oriental Electronic Co. Ltd.
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Short Abstract:

Graphene with subnanometer vacancy defects has been proposed to be effective in gas separation, catalysis, DNA sequencing and etc. The graphene samples for chemical applications are commonly synthesized by oxidative exfoliation of graphite followed by reduction and chemical functionalization. Taking fully and partially oxidized graphene as model systems, we addressed the generation and evolution of subnanometer vacancy defects by first-principles based calculations. Due to the strong exothermicity for formation of CO_2, CO, H_2O, H_2 and etc, the generation and evolution of these defects are thermodynamic driven. With the growth of O chemical potential, the generation of vacancy defects even overwhelms that of graphene oxide. The defect generation is oxygen-consuming and an O depletion region will be formed around the vacancy to fully passivate the C atoms at the vacancies with ether oxygen(-O-), carbonyl oxygen (C=O) and their combinations, when there is no environmental O supply. Further evolution of the vacancy structures would be strongly dependent on the diffusion of oxygen containing groups from O-rich region to the vacancy, which is kinetically forbidden according to our calculations. The findings paved the way for controlled synthesis of graphene samples with subnanometer vacancy defects.