Mini-symposium C2

Theoretical Exploration of Defects in and Formation Mechanism of Carbon Nanomaterials

Organizers:
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Wed - 7 Jan 2015 | 16:00 – 18:00 | 03-07, Block S16

Chair: Zhenyu Li

16:00 C2-01 Keynote
Prediction of CO₂ Capture Properties of Functionalized and Hybrid Carbon Nanotube/Graphene Structures
Xin Tan¹, Yan Jiao², Aijun Du³, Sean C. Smith⁴
¹School of Chemical Engineering, UNSW Australia, Sydney, NSW 2052, Australia; ²School of Chemical Engineering, University of Adelaide, SA 5005, Australia; ³School of Chemistry, Physics and Mechanical Engineering, Queensland University of Technology, Brisbane, Queensland 4001, Australia

16:30 C2-02 Invited
Tight-binding Molecular Dynamics Simulation Study of Defects in Graphene
Gun-Do Lee
Department of Materials Science and Engineering, Seoul National University, Seoul, Korea

17:00 C2-03 Invited
Interdependency of Subsurface Carbon Distribution and Graphene-Catalyst Interaction
H. Amara¹, R. Weatherup², F. Ducastelle¹, S. Hofmann³, C. Bichara⁴
¹LEM, ONERA-CNRS, Châtillon, France; ²Department of Engineering, University of Cambridge, Cambridge, United Kingdom; ³CINaM, CNRS, Marseille, France

17:30 C2-04 Invited
Epitaxial growth of graphene and transition metal dichalcogenides: modeling and experiments
Cecilia Mattevi
Materials Department, Imperial College London, SW7 2AZ London UK

Thu - 8 Jan 2015 | 16:00 – 18:00 | 03-07, Block S16

Chair: Feng Ding

16:00 C2-05 Keynote
Insights in the Synthesis of Carbon Nanostructures from Computer Simulation
Christophe Bichara
CINaM, CNRS and Aix Marseille University, 13288, France

16:30 C2-06 Invited
Graphene Growth on Metal Surfaces: from Mechanism Studies to Protocol Design.
Zhenyu Li
Hefei National Laboratory for Physical Science at Microscale, University of Science and Technology of China, Hefei, 230026 China

17:00 C2-07 Invited
Grain Boundaries and Chiral Edges in Graphene
Oleg V. Yazyev
Institute of Theoretical Physics, Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

17:30 C2-08 Invited
Growth Mechanism and Orientation Control of Graphene Chemical Vapor Deposition Growth
Qinghong Yuan¹, Feng Ding²
¹Department of Physics, East China Normal University, No. 500, Dongchuan Road, Minhang, Shanghai, China, 200062; ²Institute of Textiles and Clothing, Hong Kong Polytechnic University, Kowloon, Hong Kong, China
11:00 C2-09 Invited

**Defects in Carbon and Their Functional Roles**

De-en Jiang  
*Department of Chemistry, University of California, Riverside*

11:30 C2-10 Invited

**Atomistic Formation Mechanisms of Graphene on Transition Metal Substrates.**

Weicheng Zhou, Hua Chen, Wenguang Zhu, Zhenyu Zhang  
1ICQD/HFNL, University of Science and Technology of China, Hefei, Anhui 230026, China; 2Department of Physics and Astronomy, University of Tennessee, Knoxville, TN 37996, USA; 3Department of Physics, University of Texas at Austin, Austin, TX 78712, USA

12:00 C2-11 Invited

**Theoretical Exploration on the Mechanisms of Graphene Chemical Vapor Deposition (CVD) Growth**

Feng Ding  
*Institute of Textile and Clothing, Hong Kong Polytechnic University, Kowloon, Hong Kong, China*

14:00 C2-12

**Effects of Carbide Formation in Graphene Growth**

Zhunzhun Wang, Qiquan Luo, Wenhua Zhang, Zhenyu Li  
1Hefei National Laboratory for Physical Sciences at Microscale, University of Science and Technology of China, Hefei 230026, China

14:15 C2-13

**Stability and Electronic Structure of Nitrogen-Doped Graphene**

Zhuofeng Hou and Kiyoyuki Terakura  
1Department of Organic and Polymeric Materials, Graduate School of Science and Engineering, Tokyo Institute of Technology, 2-12-1 Itō-31, Ookayama, Tokyo 152-8552, Japan; 2Research Center for Simulation Science, Japan Advanced Institute of Science and Technology (JAIST), 1-1 Asahidai, Nomi, Ishikawa 923-1292, Japan

14:30 C2-14 Invited

**Combined MD/MC Simulations of Carbon Nanotube Cap Formation from Hydrocarbons and CNT Etching**

Umedjon Khalilov, Annemie Bogaerts, Erik C. Neyts  
Research group PLASMANT, Department of Chemistry, University of Antwerp, Belgium

15:00 C2-15 Invited

**Electronic and Magnetic Properties Modulation in Graphene and Graphene Hybrid Materials via Defects**

Xiaojun Wu  
*University of Science and Technology of China, Hefei, Anhui 230026, China*