Program

Advances and Applications in Carbon Related Nanomaterials: From Pure to Doping Including Heteroatom Layers

An ECI Conference

September 22-26, 2013

Gran Hotel Rey Don Jaime
Castelldefels, Spain

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Sunday, September 22, 2013

17:30 - 19:00  Conference Check-in / Registration (Hotel Lobby)
19:00 - 20:00  Welcome Drink (Terrace by the swimming pool)
20:00 - 21:30  Dinner

NOTES

• Please do not smoke at any conference functions.
• Turn your mobile telephones to vibrate or off during technical sessions.
• The location of technical sessions and poster sessions will be announced on Sunday.
• All meals will be in the hotel restaurant.
• Be sure to check your contact information on the Participant List in this program and make any corrections to your name/contact information online. A corrected copy will be sent to all participants after the conference.
Monday, September 23, 2013

07:30 - 08:50  Breakfast

08:50 - 09:00  Opening Remarks:  Raul Arenal, Chair
                Dean Miller, ECI Conferences Committee

09:00 - 11:00  **Session I: Doping of C nanotubes & graphene 1**
                Session chair: Chris Ewels

09:00 - 09:40  *Invited Talk:* Changes induced by doping on the Raman spectrum of monolayer and bilayer graphene
                Jean-Louis Sauvajol, University of Montpellier, France

09:40 - 10:00  Nitrogen-doped carbon nanotubes: Thin films, dopant identification, and electron beam damage
                Toma Susi, Aalto University, Finland

10:00 - 10:20  Fluidized bed chemical vapor deposition of nitrogen-doped carbon nanotubes for the energy storage application
                Guili Tian, Tsinghua University, China

10:20 - 11:00  *Invited Talk:* New directions toward ultra-low substitutional doping
                Paola Ayala, Vienna University, Austria

11:00 - 11:30  Coffee break

11:30 - 13:50  **Session II: Graphene 1**
                Session chair: Pierre Petit

11:30 - 12:10  *Invited Talk:* Electronic structure of a disordered grain boundary in graphene
                Philippe Lambin, University of Namur, Belgium

12:10 - 12:30  Gate modulated Raman spectroscopy of single-layer and bilayer graphene
                Riichiro Saito, Tohoku University, Japan

12:30 - 12:50  Non-covalent interactions in graphene-polymer nanocomposites
                Gregory Van Lier, Free University of Brussels, Belgium

12:50 - 13:10  Formation of grain boundary induced by electron irradiation on graphene
                Kotone Hasegawa, National Institute for Materials Science, Japan

13:10 - 13:50  *Invited Talk:* Atomically precise graphene nanoribbons
                Roman Fasel, Empa, Swiss Federal Laboratories for Materials Science and Technology, Switzerland

14:00 - 15:15  Lunch

15:15 - 17:30  *Ad hoc* sessions, discussion, free time
17:30 -18:55  **Session III: Carbon nanotubes 1**  
Session chair: Martine Mayne-L’Hermite

17:30 - 18:10  *Invited Talk: Properties of individual nanotubes with known chiral structure*  
Xuedong Bai, Institute of Physics, Chinese Academy of Sciences, China

18:10 - 18:30  **New approaches for the characterization of porous electrodes based on carbon nanotubes for oxygen reduction: From PT loaded CNT to nitrogen doped CNT**  
Henri Perez, CEA-Saclay, France

18:30 -18:50  **Bias-dependent remote joule heating by a carbon nanotube**  
Merijn Bronsgeest, University of Maryland, USA

19:00 - 20:30  **Poster Session and Social Hour**  
All posters will be kept on display throughout the conference. Participants will then be free to view/discuss posters at their convenience as well.

20:45 - 22:15  Dinner
Tuesday, September 24, 2013

07:30 - 08:45  Breakfast

08:55 - 09:00  Announcements: Raul Arenal, Chair

09:00 - 11:00  Session IV: Chacogenides 1
Session chair: Vincent Meunier

09:00 - 09:40  Invited Talk: Inorganic nanotubes and fullerene-like nanoparticles: an update
Reshef Tenne, Weizmann Institute, Israel

09:40 - 10:00  2D transition-metal dichalcogenides: Doping, alloying and electronic structure engineering using electron beam
Arkady Krasheninnikov, Aalto University, Finland

10:00 – 10:20  Novel routes to hybrid chalcogenide nanomaterials
Frank Dillon, Department of Materials, Oxford University, UK

10:20 – 10:40  Nanostructures of layered metal chalcogenides
Gotthard Seifert, Technical University of Dresden, Germany

10:40 – 11:00  NT-MDT & Renishaw (10 min. each)

11:00 – 11:30  Coffee break

11:30 – 13:30  Session V: Doping of C nanotubes & graphene 2
Session chair: Dmitri Golberg

11:30 - 12:10  Invited Talk: Nanotube-Molecular complexes for energy transfer systems
Friederike Ernst, Free University of Berlin, Germany

12:10 - 12:30  Influence of the nature of precursors and temperature on the structure and N-content in nitrogen containing carbon nanotube arrays
Martine Mayne-L’Hermite, CEA-Saclay, France

12:30 - 12:50  Bonding of nitrogen dopants in graphene
Rebecca J. Nicholls, Department of Materials, Oxford University, UK

12:50 - 13:10  Nitrogen doped single-walled carbon nanotubes: Atomic structure and configuration
Raul Arenal, University of Zaragoza, Spain

13:10 - 13:30  Nitrogen, boron and phosphorus doping in carbon nanomaterials: Insight from DFT calculations
Chris Ewels, CNRS/ University of Nantes, France

13:30 -15:00  Lunch

15:00 -18:15  Ad hoc sessions, discussion, free time
Tuesday, September 24, 2013 (continued)

18:15 – 19:15  Session VI: Chalcogenides 2
Session chair: Arkady Krasheninnkov

18:15 – 18:35  Heterostructured materials for nanoelectronics: Computational design and controlled properties
Vincent Meunier, Rensselaer Polytechnic Institute, USA

18:35 – 19:15  Invited Talk: Optical properties of graphene nanoribbons inside single-wall carbon nanotubes
Elena Obraztsova, Russian Academy of Sciences, Russia

19:15 – 20:30  Poster Session and Social Hour
All posters will be kept on display throughout the conference. Participants will then be free to view/discuss posters at their convenience as well.

20:45 - 22:15  Dinner
**Wednesday, September 25, 2013**

07:30 - 08:55  Breakfast

08:55 - 09:00  **Announcements: Raul Arenal, Chair**

09:00 - 11:00  **Session VII: Carbon nanotubes 2 + Hybrids (NP + NT or Graphene) 1**  
Session chair: Riichiro Saito

09:00 - 09:40  **Invited Talk: Electronic transport properties of functionalized metallicity sorted single walled carbon nanotubes: Gain from photoemission and XAS**  
Thomas Pichler, University of Vienna, Austria

09:40 - 10:00  **CNT-reinforced electrospun carbon fibers: Promising electrodes for energy production by enzymatic biofuel cells**  
Sophie Tingry, European Institute of Membranes, France

10:00 - 10:20  **Synthesis and potential applications of pyrolytic carbon nano-cones**  
Mathieu Delmas, CEMES-CNRS, France

10:20 - 10:40  **Modeling the encapsulation of clusters and one-dimensional crystals in carbon nanotubes**  
Eric Faulques, University of Nantes CNRS, France

10:40 - 11:00  **Controlling the nanoscale rippling of graphene with nanoparticles**  
Zoltán Osváth, Research Centre for Natural Sciences (MTA TTK), Institute for Technical Physics and Materials Science (MFA), Hungary

11:00 - 11:30  Coffee break

11:30 - 13:30  **Session VIII: Other layered nanostructures 1**  
Session chair: Philippe Lambin

11:30 - 12:10  **Invited Talk: Synthesis and heterostructures of 2D materials**  
James Hone, Columbia University, USA

12:10 - 12:30  **Lighting up excitons at defects in h-BN flakes**  
Alberto Zobelli, University of Paris Sud, France

12:30 - 12:50  **Hierarchical 1D and 2D boron nitride nanoarchitectures: Synthesis, growth mechanism and wetting properties**  
Amir Pakdel, National Institute for Materials Science (NIMS), Japan

12:50 - 13:10  **Hydroxyapatite multiwalled carbon nanotube and graphene oxide hetero-nanostructures: Integration and bioactivity**  
Jesus David Nuñez Garcia, ICB-CSIC, Spain

13:10 - 13:30  Lunch (lunch box) and visit to Barcelona

20:30 – 21:00  Reception

21:00 - 23:30  Conference Banquet
07.30 - 08:45  Breakfast

08:55 - 09:00  Announcements: Raul Arenal, Chair

09:00 - 10:55  Session IX: Hybrids (NP + NT or Graphene) 2
Session chair: Thomas Pichler

09:00 - 09:40  Invited Talk: Carbon-based materials with tailored properties: Preparation and Applications
Wolfgang Maser, CSIC-Zaragoza, Spain

09:40 - 10:00  Study of the thermal stability of supported catalytic nanoparticles for the growth of single walled carbon nanotubes with narrow diameter distribution
Pierre Petit, Institut Charles Sadron CNRS, France

10:00 - 10:20  Experimental and theoretical insights of the chemistry at the carbon nanotube supported ruthenium nanocatalysts interface
Iann Gerber, Université de Toulouse; INSA, UPS, CNRS; LPCNO, France

10:20 - 10:40  TBD  
Katya Obraztsova, Russian Academy of Sciences, Russia

10:40 -11:25  Coffee break (at Swimming Pool Terrace)

11:25 -13:05  Session X: Other layered nanostructures 2
Session chair: Raul Arenal

11:25 -12:05  Invited Talk: Atomic imaging and spectroscopy of single-layered nano-materials
Kazu Suenaga, AIST, Japan

12:05 -12:25  Atomistic simulations of nanocrystal/amorphous carbon-based composite materials
Georgios Kopidakis, University of Crete, Greece

12:25 - 12:45  Synthesis and characterisation of hetero-carbon nanotubes  
Jonathan Quinson, Department of Materials, Oxford University, UK

12:45 -13:05  Direct visualization of hierarchical nanodomains in polymer-fullerene bulk heterojunction solar cells using chromatic aberration-corrected TEM
Dean Miller, Argonne National Laboratory, USA

13:05 -13:15  Closing remarks

13:15 -14:45  Lunch and departures
1. **Nitrogen-doped single-walled carbon nanotube/graphene hybrids: Controllable synthesis, hierarchical nanostructure, and oxygen reduction performance**  
   Guili Tian, Tsinghua University, China

2. **Structural and surface properties of nitrogen doped and phosphorus doped carbon nanotubes: A comparability study**  
   Edward Nxumalo, University of Johannesburg, South Africa

3. **Synthesis of boron-substituted single-wall carbon nanotubes by arc discharge**  
   Djamel Eddine Gourari, laplace/CEMES Toulouse, France

4. **Atomic structure of ultra-long carbon nanotubes**  
   Raul Arenal, Universidad de Zaragoza, Spain

5. **In-situ KEV-ion irradiation studies on single-walled boron nitride and carbon nanotubes**  
   Raul Arenal, Universidad de Zaragoza, Spain

6. **Graphene on cobalt through chemical vapor deposition: unraveling the relation between graphene properties and the cobalt substrate**  
   Merijntje Bronsgeest, CNRS Grenoble, France

7. **Boron mediated nanotube morphologies**  
   Rebecca Nicholls, University of Oxford, UK

8. **Field-effect transistors based on WS$_2$ nanotubes with high current-carrying capacity**  
   Roi Levi, Weizmann Institute of Science, Israel

9. **Theoretical study of electronic properties of graphene on a BN monolayer substrate**  
   Rafael Martinez Gordillo, CSIC/ICN2, Spain