

Predicting new carbon nanomaterials from first principles

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Atomic scale computer modelling can be used in various ways in the field of nanomaterials science. Its role has traditionally been to support experimental work: for example discriminating between different structural models based on agreement of simulated spectra with available experimental data. Recent advances in both computer power and available algorithms mean we now have an unprecedented level of accuracy with atomic simulations, and the capability of routinely modelling extremely large scale systems containing many thousands of atoms. This allows us to move beyond confirmation of experimental findings towards realistic predictive models.

In this talk I will present some of our recent work using DFT calculations to help develop new “virtual materials”, such as two-dimensional networks of extended pi-conjugated polymers, edge control in carbon nanoribbons, and new approaches to indirect chemical doping in carbon nanotubes [1]. I will highlight ongoing collaborations with Japanese institutions, notably a new double degree programme with Toyo University [4], and links with Nagoya University (including an EU IRSES project on fluorinated nanocarbons [5]).

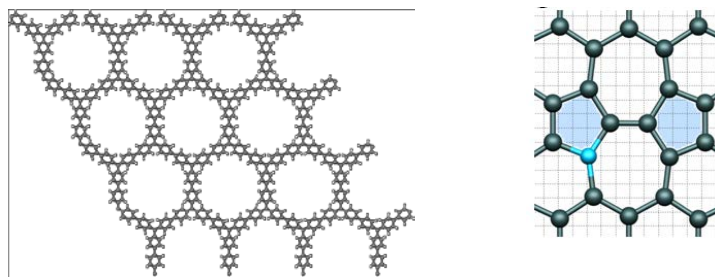


Figure: (left) 2D-network of conjugated polymers [2], (right) Substitutional nitrogen impurity in graphene, neighbouring a structural defect (5-7-7-5 “Stone-Thrower-Wales” defect) [3]

- [1] All publications available from www.ewels.info
- [2] *Dirac Cones in two-dimensional conjugated polymer networks*, J.-J. Adjizian, P. Briddon, B. Humbert, J.-L. Duvail, Ph. Wagner, C. Adda, C. Ewels, **Nat. Commun.** 5, 5842 (2014)
- [3] *Atomic Configuration of Nitrogen-Doped Single-Walled Carbon Nanotubes*, R. Arenal, K. March, C. Ewels, X. Rocquefelte, M. Kociak, A. Loiseau, O. Stephan, **Nano Letters**, 14, 5509 (2014)
- [4] <http://www.toyo.ac.jp/site/bionano/39003.html>
- [5] <http://www.nanocf.eu/index.php?id=2748&type=0&L=0>

Dr Christopher Ewels HDR



Full Time Researcher : CNRS CR1, France (since 10/2005)

Institute of Materials (CNRS UMR6502), Nantes, France

In close collaboration with experimental colleagues, I use atomic scale computer simulations to understand and design new carbon-based nanostructures with unique customised properties, either through new structural topologies or chemical and structural modification.

Refereed Publications	123	Total Publications	133
Book Chapters	6	H-index	29

Responsibilities

Coordinator Nanocarbon Transversal Action at the Institute (22 full-time researchers)

Coordinator, EU Marie Curie Training Network “Enabling Excellence” (2015-2019)

Visiting Researcher, Bio-Nano Electronics Centre, Toyo University, Tokyo, Japan (2013-2018)

Trustee (director) for the Vega Science Trust, Science Communication Charity www.vega.org.uk

Committee Member British Carbon Group (2002-), GDRI-GNT (Graphene-Nanotubes) (2008-)

Editorial advisory board, “Materials Today” (2011)

Conference co-organiser annual “NanoteC” international series (1998-2010)

Reviewer for Phys Rev, ACS, ..., regular project review for EU, PRACE, ANR (France), NSF, FNRS, ...

Previously

2003-2005 Marie Curie Individual Fellowship, Université Paris Sud, Orsay, (Christian Colliex)

2002-2003 TMR Postdoc, Composite Materials, ONERA, Paris, (Annick Loiseau)

1997-2002 2 days/week: Dept. Chemistry, Sussex University, UK (Malcolm Heggie)

1999-2002 3 days/week: The Vega Science Trust (Harry Kroto)

Charity communicating science in the media. Developed Europe’s first science TV channel broadcast over Internet. Researched programmes, production public relations.

1993-1997 PhD « Research Assistant », Physics Department, Exeter University (Bob Jones)

1989-1993 Degree BA(Hons) 2:1, Metallurgy and Materials, Keble College, Oxford University

Prizes, distinctions

- 7th British Carbon Group ‘Ubbelohde Award Lecture’ for Carbon Science (2014)
- EU Marie Curie Excellence Award (2006)

Chris Ewels graduated from Oxford University in 1993 after studying “Metallurgy and the Science of Materials”, with a fourth year at the Max Planck Institute for Powder Metallurgy. He received a Ph.D. in 1997 from the University of Exeter UK, for computational studies of oxygen defects in silicon. He then moved to Sussex University where he worked on radiation induced defects in graphite and carbon nanosystems. At Sussex he joined the Vega Science Trust with Sir Harry Kroto, where he created an online science TV channel and developed a passion for public communication of science. In Paris he worked at ONERA and was then a Marie Curie Individual Research Fellow at the Université Paris Sud within the electron microscopy group of Professor Christian Colliex. In 2006 he took up a permanent post with the CNRS at the Institute of Materials in Nantes.

His work focuses on computer modelling of point and line defects in nanoscale carbons and oxides, and he has authored over 100 journal publications including six book chapters. His interest in science communication continues, having exhibited his nanoscience art in the US (www.ewels.info) and established an award winning EU funded nanoscience web video project (www.youtube.com/nano2hybrids). In 2006 he received the European Marie Curie Excellence Award. He now runs the transversal nanocarbon action at the Institute of Materials in Nantes. His links with Japan began with a 2 month visit in 2006 to the Electron Microscopy Group of Prof. Kazu Suenaga at AIST Tsukuba. Since then he travels regularly to Japan. With Prof. Toru Maekawa he has established the first ‘double degree programme’ for exchange of PhD students between Nantes University and Toyo University’s BioNano Centre. He also collaborates with the fullerene research group of Prof. Shinohara at Nagoya, and is involved in a European network “NanoCF” with Stephen Irle at Nagoya University exploring fluorinated nanocarbon materials.