25e Congrès Général de la Société Française de Physique

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DFT Nanocarbon Modelling at IMN Nantes

Wednesday, 10 July 2019 09:30 (30 minutes)

Using **computational quantum mechanical methods** (DFT, DFTB+) and molecular dynamics we explore **carbon nanomaterials**, their atomistic, vibrational and electronic structure and structural modification, **defects** and chemical functionalisation.

- **Characterise** and understand as-grown and modified nanocarbons with experimental colleagues
- Identify and explain **commonalities** in behaviour between different nanocarbons, explore and explain their **differences**.
- Predict new nanocarbons and **nanocarbon hybrids**
- **Design new carbon-based nanomaterials** in-silico, to guide experimental colleagues

Notably we use the AIMPRO code developed by colleagues at Newcastle University, an ultra-fast Gaussian orbital based DFT code capable of routinely optimising low-symmetry systems containing hundreds to thousands of atoms (aimpro.ncl.ac.uk). This study covers a range of areas we are currently working in, in close collaboration with experimental colleagues in France, Europe, Japan and the USA, including:

- Functionalising and Filling Fullerenes
- Fullerene growth and spectroscopy
- Filling Circular and Collapsed Carbon Nanotubes
- 2D-conjugated Polymers: New Graphene-like materials
- Classifying Nanocarbons

Choix de session parallèle

Autres: Matière Condensée

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