SEMINAIRE ISMO

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Carbon (nano)structures on SiC(111) and Au(111) studied with density-functional theory

Graphene's contribution to applications promises to be huge thanks to its exotic structure: Electronically, it presents a Dirac cone at the Fermi energy, and geometrically, the honeycomb arrangement is only one atomic layer thick. In order to achieve precisely designed arrangements of graphene components a detailed understanding of its material properties is needed.

We have performed atomistic simulations of graphene structures using density-functional theory (DFT). We shall discuss the graphene layers on the semi-conducting 3C-SiC(111) surface, in particular the geometrical models of the so-called "buffer" or "zero" layer, for which no fully satisfactory geometry has been found yet. We shall review the results obtained experimentally so far, and the relaxed structure appearing from the calculations.

In addition we shall discuss the formation of graphene nanoribbons via a controlled chemical approach on a substrate [1], in the present case Au(111). We will show that it is possible to grow unique ribbons with a pre-determined edge termination with hydrogen atoms. Time permitting we shall discuss the thermodynamics of the graphene edges, as studied via DFT [2,3].

[1] "Site-specific atomically precise bottom-up fabrication of graphene nanoribbons", Jinming Cai, Pascal Ruffieux et al, Nature 466 (2010) 470-473; doi:10.1038/nature09211

[2] "Structure, stability, edge states and aromaticity of graphene ribbons", Tobias Wassmann, et al, Physical Review Letters 101 096402 (2008); doi:10.1103/PhysRevLett.101.096402

[3] "Clar's Theory, π-Electron Distribution, and Geometry of Graphene Nanoribbons", Tobias Wassmann, et al, Journal of the American Chemical Society 132 3440-3451 (2010); doi:10.1021/ja909234y

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Bât. 210 – Amphi 1 (2ème étage)

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