Centre DE Nanosciences & DE Nanotechnologies

C2N General Seminar

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"*Ab-initio quantum transport simulation of layered 2D materials-based electron devices*"

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The prediction of electronic and transport properties of nanodevices based on recently synthetized materials such as layered two-dimensional materials demands the adoption of first-principles theories to avoid the use of empirical parameters. While the use of density functional theory (DFT) for band-structure calculations is fairly established, the adoption of a full ab-initio approach for electron transport investigations has been up to now limited due to its extremely high computational cost. This talk illustrates the theory and application of a first-principles transport methodology based on the non-equilibrium Green's functions technique and employing a basis set obtained directly from the Bloch functions computed with a plane wave ab-initio solver. This enables full ab-initio quantum transport calculations with a good computational efficiency, and allows us to address self-consistent simulations of novel electronic devices. As an illustrative application, I will present an original device concept for energy-efficient, steep-slope transistors based on van der Waals heterojunctions of two-dimensional materials. In such a device, by injecting electrons from an isolated and weakly dispersive band into a strongly dispersive one, sub-thermionic subthreshold swings can be obtained, as a result of a cold-source effect and of a reduced thermalization of carriers.

Marco Pala received the physics degree and the PhD in electronical engineering from the University of Pisa, Italy in 2000 and 2004, respectively. From 2004 to 2005 he was post-doc at CEA-Leti, Grenoble, France. He entered at CNRS as research scientist in 2005 at IMEP-LAHC, Grenoble. From 2016 he is with the Centre for Nanoscience and Nanotechnology (C2N), Palaiseau, France, where is the leader of the computational electronics group. His main research interests concern the electronic and transport properties of nanoscale devices. Recently, he worked on quantum transport calculations based on ab-initio methods to assess the use of new materials in nanoelectronics.

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