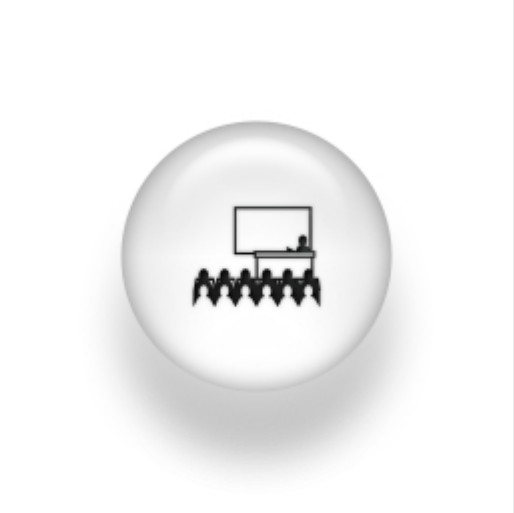
Intermolecular interaction in DFT : Application to Carbon Nanotubes and Fullerenes

Wednesday, 4 March 2009, 12:00-13.00



Dr. Y.J. Dappe
Institut de Physique et Chimie des Matériaux de Strasbourg
ABSTRACT:
A theoretical study of weak interactions in graphitic materials like Carbon Nanotubes, Fullerenes and graphene is presented here. Based on a localized orbitals DFT formalism, our treatment which has already been applied for graphene-graphene interaction describes independently the weak chemical as well as the van der Waals interaction with high accuracy. The weak chemical interaction is described in the frame of the LCAO-S2 model based on a weak overlap expansion, and the van der Waals interaction is treated in the dipolar approximation, taking into account virtual transitions of high energy. This formalism is applied here to the case of lateral interaction between CNTs, C60-dimers, adsorption of C60 on graphene and CNT, and encapsulation of C60 and CNT. The power law of the interaction is analyzed, and useful parameters like C60 coefficient and an exponential model for the “chemical” interaction are extracted. Beyond the study of graphitic materials, this work opens new perspectives in the analysis of weakly bounded metal/organics interfaces.
M.A. Basanta, Y.J. Dappe, J. Ortega and F. Flores, Europhysics Letters 70, 355 (2005).
Y.J. Dappe, M.A. Basanta, F. Flores and J. Ortega, Physical Review B 74, 205434 (2006).
Y.J. Dappe, J. Ortega and F. Flores, submitted to Physical Review B (2008).