

Avviso Di Seminario

05-12-2014, 15:00 - Aula E

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Terra' un seminario dal titolo:

"THE GROWTH OF CARBON BASED MATERIALS BY SUPERSONIC BEAM EPITAXY: EXPERIMENTS, THEORY AND CALCULATIONS "

Abstract:

Characterization of the epitaxial grown material by experimental techniques, (XPS, UPS, Auger, LEED, TEM, and Raman after the collision) demonstrates the potentiality to grow nanostructured materials at room temperature.

I also show that, in out-of-equilibrium conditions, ab-initio methods based on the Born-Oppenheimer approximation fail to capture the excited-state dynamics. Hence, we analyse the Si-and Cu-C60 collision in a non-adiabatic nuclear dynamics framework, where stochastic hops occur between adiabatic surfaces, calculated by a time-dependent density functional theory. The description of C60 impacts on metallic and semiconductor substrates is in good agreement with our experimental findings.

Il Direttore
Pasquale Lubrano