UNIVERSITÀ DEGLI STUDI DI MILANO BICOCCA

PCAM Physics and Chemistry of Advanced Materials EUROPEAN DOCTORATE

Ph.D. Course in Materials Science and Nanotechnology

University of Milano-Bicocca, Department of Materials Science, via Cozzi 55, 20125 Milano

March 7, 2018 – 11.30 a.m.

Seminar room - Department of Materials Science U5

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Tight-binding Density Functional Theory (DFTB)

an approximate Kohn-Sham DFT scheme

The foundation of the density-functional tight-binding (DFTB) method is briefly reviewed. The method is based on the density-functional theory (DFT) as formulated by Hohenberg, Kohn and Sham (KS-DFT). It is an approximate method, but it avoids an empirical parametrization by calculating the Hamiltonian and overlap matrices out of DFT-derived local orbitals (atomic orbitals - AO's). The method includes ab initio concepts in relating the Kohn-Sham orbitals of the atomic configuration to a minimal basis of the localized atomic valence orbitals of the atoms. Despite of the description of the method also some practical aspects and applications are presented.

PhD students and all interested in the seminar are kindly invited to participate.

The PhD Coordinator

Prof. Marco Bernasconi