CRETE CENTER FOR QUANTUM COMPLEXITY AND NANOTECHNOLOGY

UNIVERSITY OF CRETE
DEPARTMENT OF PHYSICS

CAPACITIES

ΓΕΝΙΚΟ ΣΕΜΙΝΑΡΙΟ ΤΜΗΜΑΤΟΣ ΦΥΣΙΚΗΣ

PHYSICS COLLOQUIUM

Thursday, 10 November 2016

17:00 -18:00

3rd Floor Seminar Room

"Electronic structure simulations for transition metal dichalcogenides"

Prof. Ioannis N. Remediakis

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Abstract

Two-dimensional materials, such as graphene and MoS2, have emerged recently as alternatives to the well-known semiconductors. These materials combine low-cost production with superb properties including low defect density, visible light photoluminescence and high carrier mobility, while they can form a variety of nanostructures including tubes, fullerenes and ribbons.

Density-Functional Theory (DFT) is routinely used to simulate the atomic and electronic structure of such materials, as well as their mechanical and electric properties. Calculations for two-dimensional materials are computationally very demanding, while multi-scale models might be necessary in order to study properties of nanostructures and composites.

In this talk, I will review the electronic structure of MoS2 and related materials and present results for the modification of the electronic density of states by introducing edge states, strain and alloying.