University of Crete
Department of Physics

Physics Colloquium

Thursday, 10 November 2022 | 17:00 – 18:00, Seminar Room 3rd floor

Investigations of materials at the nanoscale from first principles

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ABSTRACT

Ab-initio-based computational materials constitute nowadays a working horse in state-of-the-art materials science and technology. A great advantage of computational materials is that they can provide information not straightforwardly accessible by experiment, and they can identify the dominant mechanisms at the atomistic and nanoscale. In the first part of the talk we will provide a brief introduction to first-principles calculations and how these calculations can be applied to describe a large variety of materials and material's properties at different length scales. In the second part, we will formulate the problem to predict and describe a complex system embedded in and interacting with a complex environment. Specifically, we will investigate the complex interplay between surfaces and quantum mechanics at surfaces and strain energies, and their interaction with the growing environment in modern electronic and optoelectronic materials. Based on these insights, we will discuss and highlight how physics at surfaces have a strong impact on the properties of technologically important materials.