



University of Crete
Department of Physics

40 Years Anniversary Colloquium Series

Thursday, 29 March 2018 | 17:00 – 18:00, Seminar Room, 3rd floor

Realizing Dirac's vision: predictive calculations of quantum processes in semiconductors

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ABSTRACT

Paul Dirac famously observed that although “the underlying physical laws necessary for the mathematical theory of a large part of physics are completely known, the exact application of these laws leads to equations much too complicated to be soluble. It is therefore desirable to develop approximate practical methods of applying quantum mechanics to explain the main features of complex atomic systems without too much computation.” Recent advances in method development and high-performance computing have made significant progress towards realizing Dirac's vision. I will discuss how density functional theory and its extensions facilitate the approximate solution of Schrödinger's equation for interacting electrons in real materials with predictive accuracy, and the modeling of quantum processes in semiconductors. I will focus on quantum processes that govern optoelectronic materials such as phonon-mediated radiative and non-radiative recombination, and I will present results for optoelectronic materials and devices such as group-III nitrides and 2D semiconductors.