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TITLE / Τίτλος: Optoelectronic modelling of carbon-based materials and devices / Οπτοηλεκτρονικές προσομοιώσεις υλικών και διατάξεων βασισμένες στον άνθρακα

ABSTRACT / Περίληψη:

Modelling and simulation in physics and engineering has evolved from a "peculiar" intermediate between theory and experiment into a valuable and indispensable research tool. A wide range of application fields depend on computational sciences, from electronic quantum systems to fluid dynamics and weather prediction. We'll focus on recent multi-physics and multi-scale modelling approaches for **optoelectronic applications** with carbon-based materials, specifically, graphene and organic semiconductors. A variety of interesting strongly coupled phenomena emerge. Carrier dynamics in **graphene** are governed by its peculiar linear dispersion bands while its optical response is characterized by constant absorption in the visible, electrically tunable absorption in the NIR-SWIR and plasmonic excitations in the MIR-THz spectrum. A comprehensive modeling scheme of graphene-based optoelectronic applications needs to self-consistently include the optical, thermal, and electrical responses, alongside hot-carrier relaxation and electron-phonon cooling. For **organic semiconductors**, on the other hand, transport involves thermally activated hops between molecular sites. To simulate charge transport and evaluate mobility in disordered organic materials we need modelling that spans across length scales to properly describe the atomistic arrangements, the electronic interaction energies, and stochastic charge hopping. At the end, the **validation** of predictions against experimental measurements will reveal the potential of computational modelling to drive and shape the future.

BIO:

Elefterios Lidorikis is Professor of Computational Materials Science in the Department of Materials Science and Engineering at the University of Ioannina Greece. He received his BSc in Physics from Aristotle University of Thessaloniki (1993), his PhD from Iowa State University in USA (1999), held postdoctoral positions in Louisiana State University and Massachusetts Institute of Technology in US, and an industry position in the MIT spin-off Luminus Devices Inc. His research interests focus on computational nanophotonics, plasmonics and carbon-based optoelectronics.