Rice University
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Presents

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Professor

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Defect Engineering and Patterning of Crystal Surfaces, Epitaxial Thin Films, and Two-Dimensional Materials: A Computational Materials Science Approach

Defect engineering of nanomaterials and metamaterial structures, in conjunction with chemical functionalization of such materials, is a most promising route for developing new materials with unique properties and function. Moreover, the ability to control pattern formation on material surfaces by applying and precisely controlling macroscopic external forces, such as mechanical stress and electric fields, can have significant impact on improving materials function and reliability and developing innovative, directed-assembly processes for nanofabrication. Toward these goals, multiscale computational materials science has emerged as a systematic approach for developing optimal materials engineering strategies and enabling new nanomanufacturing technologies. In this seminar, we will demonstrate such computational capabilities focusing on the optimal design of two-dimensional graphene-based nanomaterials and the field-driven pattern formation on crystal surfaces and epitaxial thin films. We report results on (1) structure-property relations which can be used for precise tuning of the electronic, mechanical, and thermal properties of superstructures of diamond nanocrystals embedded between the graphene planes of twisted bilayer graphene; (2) the precisely controlled formation of multiple quantum dots (QDs), or QD molecules, by exploiting a nonlinear surface instability of coherently strained epitaxial thin films; and (3) the current-driven dynamics of single-layer islands on conducting substrate surfaces as a directed assembly strategy for surface nanopatterning. These results are based on first-principles density functional theory calculations, molecular-dynamics simulations, and self-consistent dynamical simulations according to atomistically informed continuum-scale models.

About the Speaker

Dimitrios Maroudas received his Diploma in Chemical Engineering from the National Technical University of Athens in 1987 and his Ph.D. in Chemical Engineering with a minor in Physics from the Massachusetts Institute of Technology (MIT) in 1992. He then conducted postdoctoral research at IBM's T. J. Watson Research Center in theoretical and computational materials physics. From 1994 until 2002 he was a member of the Chemical Engineering faculty at the University of California, Santa Barbara, before joining the faculty of the University of Massachusetts (UMass) Amherst in his current position as Professor of Chemical Engineering. His awards include a CAREER Award from the National Science Foundation (1995), a Camille Dreyfus Teacher-Scholar Award (1999), as well as a UMass Amherst College of Engineering Outstanding Senior Faculty Award (2009) and a UMass Amherst Faculty Exceptional Merit Award (2012). The main theme of Prof. Maroudas' research is the multiscale modeling of complex systems with emphasis on establishing materials processing-structure-properties-function relations in bulk, thin-film, and nanostructured materials that have applications in electronics, nanotechnology, and energy technologies. He has published over 225 peer-reviewed articles and given 113 invited talks and seminars. He has advised over 25 Ph.D. students and 13 postdoctoral research scholars and he is the Founding Director of the Materials Engineering Program of the UMass Amherst College of Engineering. He has served as a Director of the Materials Engineering and Sciences Division of the American Institute of Chemical Engineers (AIChE). He is currently serving on the Editorial Advisory Boards of the journals Surface Science and Materials Research Express.

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