Materials by Computational Modeling, Simulation and Theory: From Atomic Properties to Emergent Functionalities

Nadire Nayir
Karamanoglu Mehmetbey University

Abstract:
Industrial demand for low-cost synthesis and characterization of advanced materials. However, the elucidation of nucleation density, morphology, size and orientation of growth fronts on a preferred substrate are challenging and critical to the crystallinity of materials. The success and further development of sustainable advanced materials is directly linked to our ability to manipulate matter over a wide range of length scales, which has therefore required establishing a theoretical understanding of the dynamics of the growth and manipulation of materials at multiscale scale. This talk will first focus on our multiscale modeling efforts for the synthesis and characterization of low-dimensional materials. I will show some of our own results [1-4] which have been dedicated to addressing the major challenges encountered in experiments such as (i) seamless stiching of nuclei into a crystal film, (ii) impact of the surface chemistry and crystallographic structure of a substrate on the epitaxy, (iii) impact of operating conditions on the crystal structure of materials. Additionally, since technology is developing faster than ever before, and increasingly depends on constantly advancing basic research and expanding scientific knowledge, an effective-force field development for multicomponent systems has become crucial to accelerate the knowledge transfer to industry. In the second part, this talk will also provide an overview of the force fields and multiscale model framework that we developed for low-dimensional materials [5-7]. These potentials offer a computationally cost-effective and versatile research tool for the materials science community to study large-scale simulations of synthesis and defect-, phase-, strain-, and edge engineering of a material of interest, paving the way for increased application of atomic-level modeling of low-dimensional materials. In turn, new computational materials and new knowledge will benefit the society by advancing new technologies in energy conversion, storage, and other important areas.

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