

Abstract Submitted
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Defects Assisted Growth Carbon-Based Nanomaterials¹ M.N. YOON, ZHENYU ZHANG, DOUG LOWDNES, Oak Ridge National Laboratory — A multiscale approach has been applied to study the growth mechanism of carbon-based nanomaterials such as graphite flakes, fullerenes, nanotubes, and nanohorns. Especially, the role of defects during the growth of different morphologies will be discussed. At high temperatures, interesting structural transitions among given morphologies are observed when defects are introduced. The transitions are driven by entropy which plays a crucial role in determining the structural stability at these temperatures. The stability of large structures is also studied using molecular dynamics simulations and analytical calculations based on ab initio density functional techniques. We will further discuss the role of catalytic particles in determining the structural stabilities of experimentally observed nanomaterials.

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