

Abstract Submitted
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Analysis of metastable ultrasmall titanium oxide clusters using a hybrid global search algorithm and first-principles approach¹ ERIC INCLAN, Georgia Institute of Technology, Atlanta, GA 30332, JACK LASSESTER, Middle Tennessee State University, Murfreesboro, TN 37130, DAVID GEOHEGAN, MINA YOON, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831 — Research in TiO₂ materials is highly relevant to energy and device applications, however, precise control of their morphologies and characterization are still a grand challenge in the field. We developed and applied a hybrid optimization algorithm to explore configuration spaces of energetically metastable TiO₂. Our approach was to minimize the total energy of TiO₂ clusters in order to identify the energy landscape of plausible (TiO₂)_n (n = 1-100). The hybrid algorithm retained good agreement with a regression on structures published in literature up to n = 25. Using first-principles density functional theory, we analyze basic properties of the hybrid-algorithm generated TiO₂ nanoparticles. Our results show the expected convergence to bulk material characteristics as the cluster size increases in that the band gap varies with respect to the size of the nanocluster. The nanoclusters trended toward compact, low surface area structures that share characteristics of the bulk, namely octahedral microstructures as the nanoclusters increased in size. Our study helps in better identifying and characterizing experimentally observed structures.

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