Abstract Submitted
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Identification of metastable ultrasmall titanium oxide clusters using a hybrid optimization algorithm[1] ERIC INCLAN, Florida International University, Miami, FL 33174, DAVID GEOHEGAN, MINA YOON, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831 — Nanostructured TiO_2 materials have interesting properties that are highly relevant to energy and device applications. However, precise control of their morphologies and characterization are still a grand challenge in the field. Using a hybrid optimization algorithm we theoretically explored configuration spaces of energetically metastable TiO_2 nanostructures. Our approach is to minimize the total energy of TiO_2 clusters in order to identify the structural characteristics and energy landscape of plausible $(TiO_2)_n$ (n = 1-100). The hybrid algorithm includes a modified differential evolution algorithm, a permutation operator to perform global optimization on a set of randomly generated structures, and then structure refinement using a BFGS Quasi-Newton algorithm. The results were compared against known physical structures and numerical results in the literature as well as our experimentally synthesized structures. Although the global minimum became more computationally expensive to locate with increasing number of TiO_2 units, the optimizer successfully identified numerous plausible structures along a range of energies close to the global minimum energy structure for all clusters in the given range.

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