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Nanoscale phase stability reversals in titanium oxide polymorphs

PAUL KENT, Oak Ridge National Laboratory, DANIEL HUMMER, JAMES KUBICKI, Pennsylvania State University, JEFFREY POST, Smithsonian Institution, PETER HEANEY, Pennsylvania State University — A surprising discovery of nanoscience is the reversal in relative stability of materials with the same composition but different structures as particles evolve from the nanoscale to the macroscopic. These reversals can be problematic, as they frequently induce the precipitation of metastable contaminant phases during the synthesis of compounds of interest. To investigate the fundamental origins of this phenomenon, we have (1) performed a series of large scale density functional calculations to characterize the energetics of the stability reversal between rutile and anatase nanoparticles, and (2) experimentally monitored the hydrothermal crystallization of titania nanoparticles using in-situ x-ray diffraction. Although the phenomenon of stability reversal is commonly explained as a domination of the crystalline surface energy as a fraction of the total energy, we find computationally that the refined average surface structures cannot account for the stabilization of nano-anatase relative to nano-rutile, even for 3nm sized particles. Instead we find that defects associated with the edges and corners of nanocrystals contribute significantly to the energy and must be included in any description of the stability reversal.

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