Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Optical properties of TiO_2 nanoclusters MATTI ALATALO, SAMI AUVINEN, MATTI LAHTI, HEIKKI HAARIO, ERIK VARTIAINEN, Lappeenranta University of Technology, JUHO JALAVA, RALF-JOHAN LAMMINMÄKI, Sachtleben Pigments — The structural, electronic and optical properties of TiO_2 nanoclusters have been investigated using first principles calculations. The shape of the clusters is shown to affect the optical properties more than the cluster size in the ultra small particles. We show that the first principles results for the optical properties can be extended towards larger clusters by using the generalized oscillator model, fitted to the first principles data. This allows us to bridge the gap between the atomistic regime, addressable by quantum mechanical calculations up to a few nanometers, and the size region of tens of nanometers, relevant for UV applications. This method provides an extension of the turbidity spectum method, used earlier for determining the size distribution of larger TiO_2 nanoparticles. We also discuss the electronic structure of the clusters. In particular, we provide an explanation for the gap states observed in stoichiometric clusters.

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Date submitted: 03 Dec 2012 Electronic form version 1.4