Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Cluster Structure Selection Based on High Vertical Electron Affinity: The Case of TiO_2 Clusters NOA MAROM, Institute for Computational Engineering and Sciences, The University of Texas at Austin, MINJUNG KIM, Institute for Computational Engineering and Sciences and Department of Chemical Engineering, The University of Texas at Austin, JAMES CHELIKOWSKY, Institute for Computational Engineering and Sciences and Departments of Chemical Engineering and Physics, The University of Texas at Austin — We study the structure and electronic properties of $(TiO_2)_{2-10}$ clusters using basin hopping based on density functional theory (DFT), combined with many-body perturbation theory in the GW approximation. We show that in photoemission experiments performed on anions the isomers with the high electron affinity are selectively observed rather than those with the lowest energy. These isomers possess a highly reactive Ti^{3+} site. The selectivity for highly reactive clusters may be exploited for applications in catalysis.

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Date submitted: 26 Nov 2011 Electronic form version 1.4