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Self Consistent Tight Binding Study of Titanium Dioxide Nanoclusters SERKAN ERDIN, Department of Physics, Northern Illinois University, DeKalb, IL 60115 & Advanced Photon Source, Argonne National Laboratory, Argonne, IL 60439 — Here, we report our recent results on TiO_2nanoclusters in vacuum and water based on self consistent tight binding method (SCTB). We calculate the ground state energies and structures of several anatase and rutile nanoclusters of size 2-8 nm, and determine the line energy of clusters with a model described by the surface energies and Wulf-constructed shapes. Our calculations show that SCTB method describes crystallographic rutile-to-anatase phase transition in vacuum well. SCTB molecular dynamics simulation of anatase cluster in water shows the structural change of the cluster.

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