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Structure Matters More than Size: Tuning the Electronic Properties of $(TiO_2)_n$ Clusters NOA MAROM, Tulane University, New Orleans, LA, USA, SASWATA BHATTACHARYA, LUCA GHIRINGHELLI, Fritz-Haber-Institut der MPG, Berlin, Germany — To design $(TiO_2)_n$ clusters with desired properties we implemented a suite of three genetic algorithms (GA) tailored to optimize for low total energy (EGA), high vertical electron affinity (VEA-GA), and low vertical ionization potential (VIP-GA). The property-based GAs are an extension of the cascade GA reported in [1]. Analysis of the structures found by the VEA-GA and the VIP-GA vs. the EGA reveals structure-property relations. A high VEA is correlated with the presence of several dangling-O atoms (typically 3-4), rather than the previously suggested tri-coordinated Ti atom [2]. A low VIP is correlated with low bond connectivity (typically 2) between two dangling-O atoms. We show that the electronic properties of $(TiO_2)_n$ clusters with n up to 20 correlate more strongly with the presence of these structural features than with size. We further suggest that the presence of dangling-O atoms on TiO_2 clusters or surfaces may be associated with enhanced catalytic activity and that these O atoms may serve as active sites. The process of optimization for a target property reveals the underlying structure-property relations and the structural features that may serve as active sites for catalysis. This generally applicable approach may provide valuable physical insight and design rules for better nanocatalysts.

[1] S. Bhattacharya *et al.* PRL 111, 135501 (2013); N. J. Phys, in press (2014)
[2] N. Marom *et al.* PRL 108, 106801 (2012).

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