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Property-based *cascade* genetic algorithms for tailored searches of metal-oxide nano-structures SASWATA BHATTACHARYA, LUCA M. GHIRINGHELLI, Fritz-Haber-Institut der MPG, Berlin, DE, NOA MAROM, Physics and Engineering Physics, Tulane University, New Orleans, LA, USA — There is considerable interest in the computational determination of structures of atomic clusters that are detected in spectroscopy experiments. It has been suggested that in photoemission experiments performed on anions, isomers of small $(TiO_2)_n$ clusters with high electron affinity (EA) are selectively observed rather than those with the lowest energy [1]. For the theoretical modelling of these situations, searching for the energy global minimum of the potential energy surface (PES) is inefficient. By using such an approach, in fact, it is unlikely to find meta-stable isomers that have high EA or low ionization potential (IP), but energy significantly above the ground state. We present an extension to our recently developed *ab initio* cascade genetic algorithm [2], here tailored to conduct property-based (e.g., high EA, low IP) searches over the PES. The term *cascade* refers to a multi-stepped algorithm where successive steps employ a higher level of theory, and each step of the next level takes information obtained at the immediate lower level. The new algorithms are benchmarked and validated for $(TiO_2)_n$ clusters ($n = 3 - 10, 15, 20$). − [1] N. Marom *et al.* PRL **108**, 106801 (2012) [2] S. Bhattacharya *et al.*, NJP, in press (2014).

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