Automated surface structure determination with DFT

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Using density functional theory, we conduct unbiased searches for the optimum structures of stepped TiO_2(110) surfaces and Au nano-particles on flat rutile TiO_2(110). The searches employ our implementation of a genetic algorithm for structural optimization [1]. For the stepped TiO_2(110) surfaces, extra TiO_2 units are found to decorate the step edges with the Ti atoms at non-bulk positions. These structural motifs would have been difficult to identify without the automated structural search method [2]. The implications of the new step structures for adsorbates and surface reactions are discussed [3,4]. On flat TiO_2(110) the DFT calculations point to the presence of oxygen at the entire interfacial area between supported gold nano-particles and the oxide surface [5]. The interfacial oxygen atoms cover the 5-fold Ti atoms in the troughs of the (110) surface. Again, it will be stressed that the identification of this structural element is non-trivial and strongly rely on the use of the automated structural search method. A 24 atom Au cluster is optimized with the same methods and its activity towards the CO_2 formation from CO and oxygen is studied and comparisons are made for various edge and corner sites showing a large variation in the local chemical activity[6].

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