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Study of Au/TiO_2 interface structure using Energy Density Method MIN YU, DALLAS R. TRINKLE, RICHARD M. MARTIN, University of Illinois, Urbana-Champaign — We propose a way to decompose the total energy in a material into the contribution associated with each of the atoms, using the first principles energy density formalism[1]. Although the energy density function is non-unique up to a gauge transformation, we show that unique defect energies can be found by defining volumes for each atoms using the Bader charge analysis[2]. The methods are applied to gold nanoclusters supported on rutile titanium dioxide, which are commonly used as catalysts for chemical reactions. The variation in structure and chemistry of the interface may affect catalytic acticity. In this work, we study four model interfaces; $Au(111)//TiO_2(110)$ and $Au(100)//TiO_2(110)$, with and without bridging oxygen. Calculations are performed using the projector augmented wave method implemented in the Vienna ab initio simulation package[3], and the energy density method computes the interfacial energies to determine the equlibrium interfacial structure. [1]Phys. Rev. B 45, 6074 (1992) [2]Comput. Mater. Sci. 36, 254 (2006) [3]Phys. Rev. B 59, 1758 (1999)

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