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Structure and stability of stepped Au(111)/TiO_2(110) interface
BORA LEE, DALLAS R. TRINKLE, Department of Materials Science and Engineering, University of Illinois, Urbana-Champaign — Au nanoparticles supported on TiO_2 surfaces has been widely studied due to its interesting catalytic properties. However, the Au/TiO_2 interface possesses a complex structure, making property determination difficult. In this study, Au layers on TiO_2 support associated with complex step structure have been investigated using energy density method (EDM) based on density functional theory. EDM provides the energy for each of atoms. This allows analysis of structure stability from the changes in atomic energy and work of adhesion is evaluated without spurious error, which leads accurate energy of complex interface structure of Au/TiO_2 with step configuration. We examine the changes with a stepped TiO_2 and Au surfaces; in particular, steps on surfaces of (110) TiO_2, (1x1) reduced surface and (1x2) added-row reconstructed surface, and both (001) step microfacet and with (111) step microfacet of Au (111) surfaces are considered. EDM results indicate that the step structure energy is localized, showing a large energy variation within one unit cell. The relaxed geometry of stepped interface Au/TiO_2 is consistent with the experimentally observed result with transmission electron microscopy. The detailed analysis including the charge density and electronic structures will be presented.

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