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Highly stable bimetallic AuIr/TiO2 catalyst: physical origin of the intrinsic stability against sintering. ERNESTO MARINERO, CHAN WAN HAN, School of Materials Engineering, Purdue University, PAULAMI MAJUNDAR, School of Chemical Engineering, Purdue University, ANTONIO AGUILAR-TAPIA, RODOLFO ZANELLA, CCADET, Universidad Nacional Autonoma de Mexico, JEFFREY GREELEY, School of Chemical Engineering, Purdue University, VOLKAN OTARLAN, School of Materials Engineering, Purdue University —
It has been a long-lived research topic in the field of heterogeneous catalysis to find a way to stabilizing supported Au catalysts against sintering. Herein, we report highly stable AuIr bimetallic nanoparticles on TiO2 synthesized by sequential deposition-precipitation. To understand the physical origin of the high stability AuIr/TiO2 system, we have used scanning transmission electron microscopy (STEM), STEM-tomography and density functional theory (DFT) calculations. 3D structures of AuIr/TiO2 obtained by STEM-tomography indicate that AuIr nanoparticles on TiO2 have intrinsically lower free energy and less driving force for sintering than Au nanoparticles. DFT calculations on segregation behavior of AuIr slabs on TiO2 showed that the presence of Ir near the TiO2 surface increases the adhesion energy of the bimetallic slabs to the TiO2 and the attractive interactions between Ir and TiO2 lead to higher stability of the AuIr nanoparticles compared to Au nanoparticles.

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