Effect of the support on the electronic structure of Au nanoparticles supported on transition metal carbides: Choice of the best substrate for Au activation

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Periodic density functional theory calculations on large supercells have been carried out to investigate the atomic and electronic structure of small gold particles (Au2, Au4, Au9, Au13, and Au14) supported on the (001) surface of various transition metal carbides (TiC, ZrC, VC, and ?-MoC). All the supported Au particles exhibited strong interactions with the C sites of the metal-carbide surfaces. Nevertheless, the interactions between adsorbed Au atoms were attractive, thus ultimately facilitating nucleation of two- or three-dimensional metal particles. The presence of the underlying carbide strongly modified the electronic structure and charge density of the supported metal particles resulting in the experimentally proven improved catalytic performance of the resulting systems as compared with cases where the support is an oxide. The electronic perturbations were quite strong for two-dimensional gold particles directly in contact with the carbide substrates and gradually decreased fo