Understanding Catalytic Materials at the Molecular Level:

From Thermal Chemistry to Photochemistry

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The main emphasis of this talk will be monitoring catalytic reaction mechanisms using in-situ experimental techniques at the molecular level. The first genre of catalysts to be discussed is TiO_2-promoted NO_x-Storage Reduction (NSR) catalysts for automotive emission control applications, which function through thermally activated surface processes[1-5]. Experimental results from ultra-high vacuum (UHV) applications on atomically well-defined planar model catalysts as well as realistic high-surface area (mesoporous) materials will be combined with theoretical Density Functional Theory (DFT) modeling results. Through these results, surface functionalization of conventional NSR materials (i.e. BaO/Al_2O_3) with TiO_2 is presented as an effective strategy to "fine-tune" the surface dispersion of the catalytically active nano-domains, obtain superior NO_x storage capacity and enhance tolerance against catalytic sulfur poisoning. Inspired by the thermally-activated automotive catalysts given above, a new genre of photochemically-activated TiO_2-promoted $DeNO_x$ catalysts will also be introduced. These novel photochemically activated systems called "Photocatalytic NOx Oxidation and Storage" (PHONOS) systems, operate under ambient conditions (25 °C) and offer a hybrid platform combining thermal catalysis and photocatalysis.[6] I will also briefly mention our recent mechanistic studies on H_2 generation from formic acid using an extremely selective and active heterogeneous catalytic architecture[7] and model catalyst studies on oxidative coupling of alcohols to esters over the Au(111) model catalyst surface[8].

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