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SURFACE SCIENCE APPROACH TO THE MOLECULAR LEVEL INTEGRATION OF THE PRINCIPLES IN HETEROGENEOUS, HOMOGENEOUS AND ENZYME CATALYSIS

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The surface science of chemical reactivity utilized single crystal surfaces to determine the atomic structures at interfaces responsible for rearrangements of molecules through changes at covalent or charge transfer (acid-base) bonds. The evolution of nanomaterials science has had a large impact on molecular catalysis science since most heterogeneous, homogeneous and enzyme catalysts are nanoparticles in the 0.8–10 nm range. Monometallic and bimetallic nanoparticles as well as core-shell structures and oxide-metal interfaces are used to study multipath catalytic reactions with high product selectivity. At the same time instruments were developed that can be employed to study catalysts under reaction conditions to monitor dynamic changes that occur during catalytic reactions, their atomic and molecular structure, and composition and oxidation state with high spatial and time resolution. These *in-situ* surface techniques include sum frequency generation vibrational spectroscopy, high pressure scanning tunneling microscopy along with synchrotron techniques of X-ray spectroscopies. Discoveries have included the size and shape dependence of turnover rates and product selectivity and other kinetic variables, the importance of oxide-metal interfaces in heterogeneous catalysis and the dominance of covalent bond and charged ion chemistry in transition metal and acid-base catalysis. Below 2 nm the metal nanoparticles have electronic structures that stabilize charge states, which can be used to heterogenize homogeneous catalysts. Enzymes can be immobilized on a DNA to aniline functionalized glass and they maintain most of their catalytic activity in this mode. Our aim is integration of the three fields of catalysis, heterogeneous, homogeneous and enzyme by developing hybrid systems and new instrument that permit studies of increased catalytic complexity.