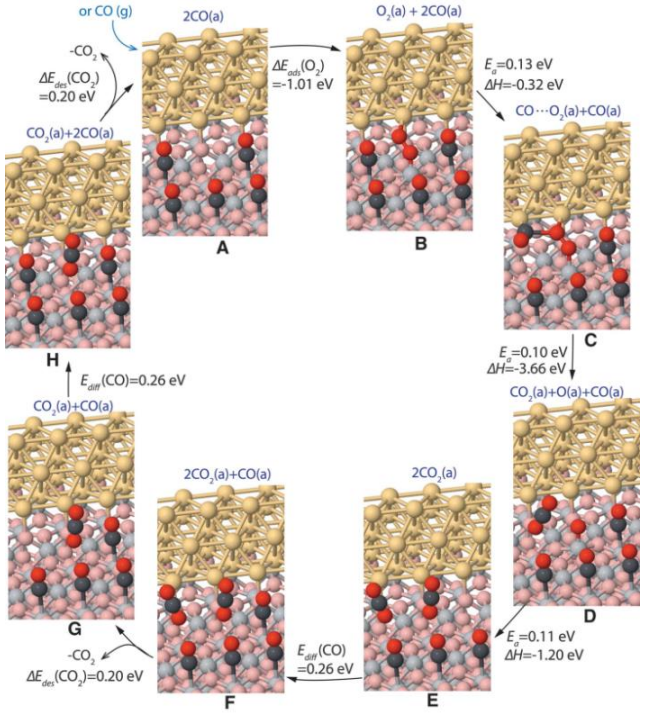

Our research program is focused on modeling the atomic features and molecular phenomena that govern catalysis and materials processing. We are using computational chemistry and molecular reaction modeling to examine the properties and performance for a wide range of different material including metals, bimetallics, metal oxides and zeolites for memory device fabrication. The performance of these materials depends on their atomic surface structure and composition. The chemistry and kinetics at a solid-fluid interface are controlled by chemical bonding between the adsorbates and the surface as well as the environment at the active site.

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"The integration of theory and simulation to design surfaces, reaction environments, and proton-coupled electron transfer systems that mimic enzymes in the transformation of molecules."

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