Molecular Activation
induced by
Single Atomic Metal Anions and Metal Hydride Anions
and a progress report on
Cluster Models of Single Atom Catalysts

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We report on the molecular activation of carbon dioxide, methane, water, and hydroxylamine by several single atomic metal anions, i.e., Pt^-, Pd^-, Ni^-, Au^-, and Ir^-, and by two metal hydride anions, i.e., PdH^- and $PdCuH^-$, using a synergetic combination of anion photoelectron spectroscopy and computations, the latter provided by theoretical partners. While some of these studies involved binary combinations of the above anions and the above molecules, an example being the activation and hydrogenation of CO_2 by PdH^-, others involved tertiary combinations of the above anions and two different molecules, an example being the simultaneous functionalization of CH_4 and CO_2 by Pt^-.

We also report on progress forming and studying the reactions of cluster models of single atom catalysts (SAC). These species have the stoichiometries, $M'(MO)_n$, where M' is a single metal atom site on the exterior of a metal oxide cluster, $(MO)_n$, thus mimicking single atom catalyst sites on surfaces. Using a magnetron source, we have made many different compositions of $M'(MO)_n^+$ cluster cations and soft landed them onto substrates, where they loss their charge and became neutral SAC models. Progress is discussed. In parallel with our experiments with single atomic metal anion activation, we have also prepared anionic versions of $M'(MO)_n^-$ model SAC clusters. Progress is discussed.