# Getting more bang for your buck:
# Fully relaxed electronic states and folding in larger basis set effects with exponential parameterizations

Thomas Watson Jr.
*Department of Chemistry*
*Princeton University, Princeton, NJ 08455*

Coupled cluster (CC) theory is the method of choice (when feasible) for quantitative information about the electronic structure of molecules in "well-behaved" electronic states. It is capable of achieving chemical accuracy when limited to single and double substitutions with a perturbative treatment of triples for the ground state (CCSD(T)) and for singly-excited states via the equation of motion framework (EOM-CCSD(T)).

Rather than use CC methods primarily for the direct determination of the correlation energy, we will describe a variational CC method capable of determining fully relaxed electronic states – with applications to ionization potentials – and we will describe the use of canonical transformations to "fold in" high-energy excitations to the virtual space into a smaller basis set.