COMPUTATIONAL STUDIES OF THE ELECTRONIC SPECTRA OF TRANSITION-METAL-CONTAINING MOLECULES

JAMES T. MUCKERMAN, ZHONG WANG, TREVOR J. SEARS[a], *Chemistry Department, Brookhaven National Laboratory, Upton, NY 11973-5000*; and HUA HOU, *Chemistry Department, Wuhan University, Wuhan, P.R. China*.

We have carried out *ab initio* multi-reference configuration interaction (MRCI) and other post-Hartree-Fock calculations of the low-lying electronic states of several transition-metal-containing molecules. We will present examples of this work that illustrate interesting features and/or technical difficulties. Beginning with diatomic molecules, we will discuss the electronic states of iron and vanadium monohydride, FeH and VH. It is well known that it is very difficult to obtain the correct ordering of the $^4\Delta$ and $^6\Delta$ states of FeH even with very high-level calculations, so the purpose of the FeH study was to calibrate our methodology against the large body of experimental data on that system in order to make reliable predictions about the relatively unknown spectrum of VH. Electronic properties of the triatomic species TiC_2 include a nested group of low-lying triplet states (including the electronic ground state) that exhibit conical intersections that may be accessible to the vibrational ground state. For the much larger titanium metcar, Ti_8C_{12}, we will discuss the problem of identifying the ground electronic state.

[a]Work at Brookhaven National Laboratory was carried out under Contract No. DE-AC02-98CH10886 with the U.S. Department of Energy and supported by its Division of Chemical Sciences, Office of Basic Energy Sciences.