EXCITED STATES OF THE DIATOMIC MOLECULE CrHe

JOHANN V. POTOTSCHNIG, MARTIN RATSCHEK, ANDREAS W. HAUSER and WOLFGANG E. ERNST, *Institute of Experimental Physics, TU Graz, Petersgasse 16, 8010 Graz, Austria*.

Chromium (Cr) atoms embedded in superfluid helium nanodroplets ($He_N$) have been investigated by laser induced fluorescence, beam depletion and resonant two-photon ionization spectroscopy in current experiments at our institute. Cr is found to reside inside the $He_N$ in the $a^7S$ ground state. Two electronically excited states, $z^7P$ and $y^7P$, are involved in a photoinduced ejection process which allowed us to study Fano resonances in the photoionisation spectra[a]. The need for a better understanding of the experimental observations triggered a theoretical approach towards the computation of electronically excited states via high-level methods of computational chemistry. Two well-established, wave function-based methods, CASSCF and MRCI, are combined to calculate the potential energy curves for the three states involved. The character of the two excited states $z^7P$ and $y^7P$ turns out to be significantly different. Theory predicts the ejection of the Cr atom in the case of an $y^7P$ excitation as was observed experimentally[b]. The quasi-inert helium environment is expected to weaken spin selection rules, allowing a coupling between different spin states especially during the ejection process. We therefore extend our theoretical analysis to the lowest state in the triplet- and quintet- manifold. Most of these alternative states show very weak bonding of only a few $\mathrm{cm}^{-1}$.

[a] A. Kautsch, M. Hasewend, M. Koch and W. E. Ernst, Phys. Rev. A 86, 033428 (2012).
[b] A. Kautsch, M. Koch and W. E. Ernst, J. Phys. Chem. A, accepted, doi:10.1021/jp312336m