

## UNDERSTANDING $\text{UO}_2^+$ BY MODELING ELECTRONIC AND VIBRATIONAL SPECTROSCOPY

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Spin-orbit configuration interaction (*SO-CI*) continues to be a valuable electronic structure tool in understanding the electronic states of small actinide containing molecules.<sup>[1]</sup> Recent interest has a variation of a familiar actinide molecule,  $\text{UO}_2^+$ . The additional electron would appear to be a simple alteration or perturbation to an understood system, but experimentally it presents some questions for theory to investigate. Principal questions involve characterization of the lowest electronic states in  $\text{UO}_2^+$  involves occupation of the either the  $5f_\phi$  or the  $5f_\delta$  non-bonding orbitals and some simple excitation generates a multitude of electronic states. Use of self-consistent field with improved virtual orbital calculations (*SCF*) will again be the foundation of the *SO-CISD* determination of the potential energy surfaces (*PES*) of the ground and low lying excited states of the  $\text{UO}_2^+$  molecule. *PES* evaluation will occur along the internal coordinates of  $r_{\text{UO}}$  and  $\theta_{\text{LOUO}}$ , and will be variationally fit to determine bound vibrational levels present within the ground and low-lying excited states. Vibrational and electronic energy levels should help clarify and describe new and interesting spectra and other properties.

<sup>[1]</sup>Gibson, J. K.; Haire, R. G.; Marcalo, J.; de Matos, A. P.; Mrozik, M. K.; Pitzer, R. M.; Bursten, B. E. *Organomet.* **2007**, 26(16), 3947–3956.