

# Computing@PNNL SEMINAR

## *C–C Bond Formation of Mg and Zn Activated Carbon Dioxide*

**Einar Uggerud, Ph.D.**

Hylleraas Centre for Quantum Molecular Sciences  
Department of Chemistry, University of Oslo



**January 12 | 3 PM | EMSL 1077**

Gas phase activation of  $\text{CO}_2$  by chloride tagged metal atoms,  $\text{CIM}^-$  ( $\text{M} = \text{Mg}, \text{Zn}$ ), has been investigated by mass spectrometry and high-level quantum chemistry. Both metals activate  $\text{CO}_2$  with significant bending of the  $\text{CO}_2$  moiety to form complexes with the general formula  $[\text{CIM}, \text{CO}_2]^-$ . The structure of the metal- $\text{CO}_2$  complex depends on the method of formation, and the energy landscapes and reaction dynamics have been probed by collisional-induced dissociation and thermal ion molecule reactions with isotopically labelled species. Having established these structural relationships, Professor Uggerud's work examines the gas phase reactivity of  $[\text{CIM}(\kappa^2\text{-O}_2\text{C})]^-$  with acetaldehyde (here considered a carbohydrate mimic). Formation of lactate and enolate-pyruvate complexes are observed, showing that  $\text{CO}_2$  fixation by C–C bond formation takes place. For  $\text{M} = \text{Zn}$ , even formation of free pyruvate ( $\text{C}_3\text{H}_3\text{O}_3^-$ ) can be observed. Professor Uggerud will discuss implications of the observed  $\text{CO}_2$  reactivity to electrochemical conversion of  $\text{CO}_2$ , as well as to biochemical and artificial photosynthesis. He also will share detailed potential energy diagrams obtained by the quantum chemical calculations that offer models consistent with experimental observation.

Professor Uggerud will be onsite and available by appointment at PNNL on January 09-12, 2018. For more information, contact **Sotiris Xantheas**.