Center for Molecular Spectroscopy and Dynamics, IBS-Korea University

IBS Center for Molecular Spectroscopy and Dynamics

Seminar

- **SPEAKER**
  Dr. Sohn So Hyeong (IBS CMSD)

- **TITLE**
  Bond formation dynamics of dicyanoaurate in the excited state

- **ABSTRACT**
  Because the chemical bond formation and breaking play crucial roles in determining the characteristics of the material, it is necessary to identify the simple but decisive process to understand the chemical reactions. Gold complexes, the suitable system for observing bond formation dynamics, have attracted great attention from many researchers for its nature, aurophilicity, making gold atoms aggregate themselves. A trimer of dicyanoaurate ([Au(CN)2-]3) is non-covalently bound in the ground state as other gold complexes and has a loose and bent structure. Upon photoexcitation, however, structural changes including bond contraction occur, resulting in a tight and linear staggered structure with covalent bonds in the excited state.

  Time-resolved spectroscopy has been regarded as one of the best techniques, enabling to track the bond formation dynamics upon photoexcitation in real time. The femtosecond time-resolved luminescence (TL) was employed, which provides exact elucidation by obtaining the excited state dynamics of [Au(CN)2-]3 in the S1 state selectively without further signal reconstruction to derive a final conclusion of the bond formation process. Indeed, it was successfully clarified that the bond formation process using the precisely obtained reaction time constants and the coherent wave packet oscillation with high time resolution. Upon photoexcitation to S1, the intersystem crossing occurs within <20 fs due to the large spin-orbit coupling followed by the structural change in 1.5 ps. Subsequently, the higher oligomer is formed within 1 ns. TL and TL spectra reveal a strong coherent excitation of the symmetric Au–Au stretching vibration at 74 cm-1 through the non-Condon effect.

- **DATE AND VENUE**
  May 20, 2020 (Wednesday, 5:00 - 6:00)
  Seminar Room B (119), KU R&D Center

- **LANGUAGE**
  Korean