Carnegie Mellon
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"Controlling Gold Nanoclusters with Atomic Precision"

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Ligand-protected metal nanoclusters with a specific number of atoms in the particle (M_nL_m *n*=the number of metal atoms, typically <2 nm) possess fundamentally different electronic and optical properties from those of larger crystalline nanoparticles (i.e. nanocrystals). Gold thiolate nanoclusters $Au_n(SR)_m$ are of particular interest due to their excellent chemical stability and elegant optical properties. However, synthesizing $Au_n(SR)_m$ nanoclusters with atomic precision remains a major challenge, which significantly hampers the pursuit of fundamental studies of this new type of material and further development of their practical applications. In this talk, I will present our recent progress in the synthesis and studies of properties of atomically precise $Au_n(SR)_m$ nanoclusters (*n* ranging from a few dozens to hundreds). Unlike crystalline Au nanoparticles (typically > 2 nm)—which are large enough to exhibit fcc crystallinity (with translational symmetry), $Au_n(SR)_m$ nanoclusters do not exhibit such an atomic packing structure. Indeed, a new type of noncrystallographic atomic packing mode has been discovered in our recent X-ray crystallographic work on $Au_{25}(SR)_{18}$ and $Au_{38}(SR)_{24}$ nanoclusters. DFT calculations, coupled with experiments, have revealed quantized electronic structure and intrinsic magnetism in such nanoclusters. These nanoclusters also have been demonstrated to be excellent catalysts for selective oxidation and hydrogenation processes. Correlation of $Au_n(SR)_m$ crystal structure and catalytic properties may eventually provide a fundamental understanding of gold catalysis.

Rongchao Jin received his B.S. degree (in Chemical Physics) from the University of Science and Technology of China (USTC) in 1995. After graduation, he was admitted to the Graduate School of the Chinese Academy of Sciences, and joined the research group of Professor Wenzhao Li at Dalian Institute of Chemical Physics (DICP), where he conducted research on the catalytic conversion of natural gas to synthesis gas on Ni and noble metal heterogeneous catalysts. He obtained his M.S. degree in 1998. In 1999, he came to Northwestern University (Illinois, USA) to pursue his Ph.D. degree, where he worked with Prof Chad A. Mirkin and Prof George C. Schatz. His doctoral thesis research focused on noble metal nanocrystal syntheses, optical property studies, and development of biological applications. He obtained his Ph.D. degree in 2003, and then worked at the University of Chicago (Illinois, USA) as Research Associate with Prof Norbert F. Scherer and studied femtosecond laser excited second harmonic generation (SHG) from single metal nanoparticles. In the fall of 2006, he joined the chemistry faculty of Carnegie Mellon University (Pennsylvania, USA). His current research interests are atomically precise nanoparticles, optics and catalysis.