WHEN MOLECULES BECOME METALS

A major challenge in nanoscience concerns understanding behaviour of systems when their size increases from a few atoms towards bulk. The properties of small molecules and bulk matter are well understood while nanoclusters and small particles need to be studied much more to uncover their size-dependent properties. Nanometer-scale, ligand-stabilized metal clusters have emerged in recent years as a novel form of nanoscale matter with potential applications in molecular electronics, optics, sensing, drug delivery and biolabeling. Tremendous advances have been achieved in discovering their structures due to contributions from synthetic work, mass spectrometry, X-ray crystallography, atomic-resolution microscopy and density functional theory computations. The total number of reported stable compositions and/or structures is now of the order of 150. It is now well established that the smallest sub-nanometer clusters can be characterized by the same terms as one conventionally uses to characterise molecules, that is, they have discrete quantized electronic and optical properties, a well-defined HOMO – LUMO energy gap, and so on. The largest structurally known clusters have metal cores of 3-4 nm, show an (almost) continuous density of electron states, a closing HOMO-LUMO gap, and feature plasmonic optical absorption. This talk discusses recent progress in understanding the cross-over region of these clusters where “molecules” become “metals”.