DEPARTMENT OF CHEMISTRY AND ENVIRONMENTAL SCIENCE
SEMINAR SERIES
SPRING 2018

DATE: TUESDAY, FEBRUARY 15, 2018

WHERE: ELECTRICAL AND COMPUTING ENGINEERING DEPARTMENT - 202

TIME: 1:30PM

GUEST SPEAKER

Dr. Zhenfei Liu

TOPIC

On the border between molecules and solids: Level alignment and level broadening

ABSTRACT

Many physical processes in nanoscience that impact device function take place at the interfaces between molecules and metal electrodes. Among all kinds of interfaces, single-molecule junctions provide excellent testbeds for understanding the electronic structure and charge dynamics at metal-organic interfaces that are representative of those in energy-conversion applications. In this talk, I will introduce two concepts, level alignment and level broadening at metal-organic interfaces, which characterize the electronics structure of molecular resonance at interfaces and determine charge dynamics.

In the first part, I will introduce methods that I developed to correct the errors of conventional density functional theory (DFT) in level alignment, based on many-body perturbation theory. The methods are applied to single-molecule junctions and lead to a quantitative agreement with experiments in transport properties. In the second part, I will introduce a method to extract the phenomenological level broadening from non-equilibrium Green's function calculations. The method is applied to both symmetric and asymmetric single-molecule junctions and leads to the understanding of transport behaviors in terms of molecular orbitals.

Committee members:
Dr. Lev Krasnoperov, Dr. Alexei Khalizov, Dr. Yong Yan