

# Center for Quantum Science and Engineering (CQSE)

Weekly Seminar  
May 6, 2011 (Friday)

TIME May 6, 14:30 ~ 15:30  
TITLE Electrical Transport through Single-Molecule Junctions  
SPEAKER Dr. Chao-Cheng Kaun 關肇正博士  
Research Center for Applied Sciences, Academia Sinica  
PLACE Rm716, CCMS & New Physics Building, NTU

## Abstract

Using first-principles calculations based on the density functional theory and the nonequilibrium Green's functions approach, we study the charge transport in Au-alkanedithiol-Au single-molecule junctions with different electrode orientations and molecular lengths. We attribute the recently measured high-/low-conductance in these heterostructures to two distinct electrode orientations, [100] and [111], which can control the electrode-molecule coupling as well as the tunneling strength by way of diverse band structures. Our detailed analysis on the transmission spectra suggests that even a single alkanedithiol junction can serve as a double quantum-dot system to yield tunable quantum interference.

