

# Joint CQSE and CASTS Seminar

**Weekly Seminar**  
**Mar. 1, 2013 (Friday)**

**TIME** Mar. 1, 14:30 ~ 15:30  
**TITLE** Thermoelectric Properties of Nanoscale Junctions and Their Possible Device Applications  
**SPEAKER** Prof. Yu-Chang Chen  
Department of Electrophysics, National Chiao Tung University  
**PLACE** Rm716, CCMS & New Physics Building, NTU

## Abstract

Density-functional theory (DFT) combined with Lippmann-Schwinger equation(LS) has been widely applied to investigate non-equilibrium electron transport and thermoelectric properties of the nanoscale junctions. In this talk, we will briefly present an introduction for DFT+LS theory for the nanoscale junctions formed by atoms/molecule sandwiched between bimetallic electrodes (modeled as electron jellium) with semi-infinite planar surfaces. We then focus on how we apply LS+DFT to investigate the thermoelectric properties of nanojunctions in response to temperatures, biases, gate voltages, and electron-vibration interactions from first-principles approaches. We propose several thermoelectric nano-devices, such as atomistic refrigerators, power generators, and self-powered transistors, and also discuss their device theories.

