# Joint CQSE and CASTS Seminar

## Weekly Seminar
## Mar. 21, 2014 (Friday)

TIME Mar. 21, 14:30 ~ 15:30
TITLE Atomistic Modeling of Single-Molecule Conductance
SPEAKER Prof. Chao-Cheng Kaun
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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 demonstrate that single-molecule junctions can be constructed by chiral single-wall gold nanotubes, which display different transmission spectra from the ones based on achiral gold nanowires. The character of the molecule features the main conduction channel, determining the distribution of local density of states, which can be controlled further by the chirality of the electrodes. Calculated conductance values being in good accord with the available measured data indicates that our analysis can shed light into the viable junction geometries and their conduction mechanisms.