

# Joint CQSE and CASTS Seminar

Weekly Seminar  
Oct. 28, 2016 (Friday)

TIME Oct. 28, 2016, 14:30 ~ 15:30  
TITLE Computational Modeling of Nanoelectronics  
SPEAKER Prof. Chao-Cheng Kaun  
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## Abstract

Using first-principles calculations, we study electronic properties of device-related nanostructures. For example, conductance superposition rule in carbon nanowire junctions with parallel paths is demonstrated, providing an understanding on all  $\pi$  conjugated systems for designing efficient nanoelectronic devices. Conductance of a double-barrier single-molecule junction, consisted of a molecule on an insulating surface with a STM tip, is analyzed, revealing a key to control the gate leaking current in nanoscale transistors. In addition, quantum well states and the magnetic interlayer exchange coupling (IEC) in the Fe/Ag/Fe trilayer are investigated, showing that the ferromagnetic-layer thickness crucially impacts the IEC oscillation in magnetic trilayers through quantum resonances. This result readily explains the recent experimental finding and provides a new degree of freedom to efficiently tune the magnetic coupling in recording materials and to eliminate recording noises.

