

Joint CQSE and CASTS Seminar

2018
Nov. 30, Friday

TIME Nov. 30, 2018, 14:30 ~ 15:30
TITLE Computational Modeling of Quantum Resonances in Nanostructures
SPEAKER Prof. Chao-Cheng Kaun
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Abstract

Many electronic and magnetic properties of nanostructures are driven by quantum-well resonances, for examples, the conductance of molecular junctions and the magnetization of thin films. Using first-principles calculations, we address resonant-related quantum transport in single-molecule junctions, consisting of the molecules, such as alkanedithiol, benzenedithiol, and peptide, contacted with Au electrodes. For the magnetic thin films, we correlate quantum well states with the magnetic interlayer exchange coupling in Fe/Ag/Fe trilayers, and with the magnetic anisotropy in Fe/Ag films, predicting that the magnetization orientation of a particular thick Fe film can be switched electrically.

