Micro&Opto Electronics Seminars

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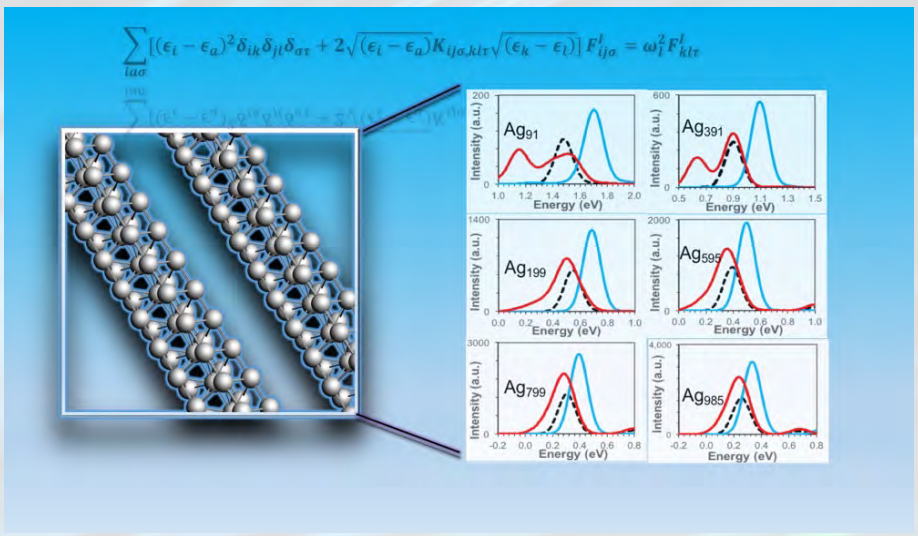
Quantum Plasmonics with Approximate TD-DFT Methods

by Asst. Prof. Fahri Alkan

Abstract

Noble metal nanoparticles exhibit unique optical properties as a result of their surface plasmon resonance (SPR) property. Theoretical treatment of SPR includes methodologies ranging from classical Mie theory to ab initio methods such as DFT. The classical methods often provide useful information for larger systems ($r \geq$ 10nm), however, they become problematic for cases where the quantum effects become dominant. In such cases, DFT and other ab initio methods can be employed to investigate the quantum nature of the system. However, the application of these methods are usually feasible for systems with 200-300 atoms, and approximations are often needed for larger nanoparticles.



In this talk, we will look into quantum effects on the SPR, which are investigated with TD-DFT and approximate TD-DFT methods, particularly for the emerging SPR modes in plasmonic assemblies with subnanometer gap distances. Quantum mechanical origin of SPR modes in such systems will be explored from a configuration-interaction perspective. Furthermore, the accuracy and efficiency of approximate density functional tight-binding (DFTB) and time-dependent DFTB (TD-DFTB) methods for the prediction of optical and electronic properties of nanoparticles will be discussed for different particle sizes (20-2000 atoms) and different inter-particle distances. Finally, we will assess the current trends in approximate TD-DFT methods (such as DFT+TB and sTD-DFT) and their applications to plasmonic systems.

Date and Time: 19 November 2019, 15:00

Place: CRF Seminar Room