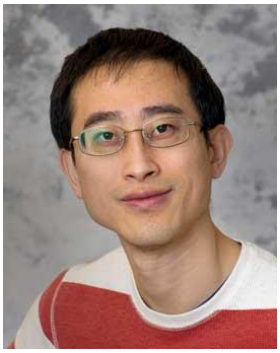
Special Seminar

THE INSTITUTE FOR MOLECULAR ENGINEERING

Wednesday, November 2nd at 11:00

Eckhardt Research Center , Room 201B



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First Principles Modeling of Electronic Excitations for Materials Applications

Electronic excitations are fundamental physical processes. Spectroscopic information, including absorption and emission spectra, from electron or photon probes is crucial for materials characterization and interrogation. When experimental data are supplemented and interpreted by first principles atomic modeling, a coherent physical picture can be established to provide physical insights into the intriguing structure-property-function relationship of functional materials.

In this talk, the importance of the first principles modeling of electronic excitations is highlighted with three examples. In the first example, we investigated the oxygen 1s core- level binding energy shift of bilayer silica films on Ru(0001) under different surface oxygen coverages in the X-ray photoelectron spectroscopy (XPS) measurement. In the second example, we raised the question on an inverse problem: how to solve the underlying local structural arrangements from observed spectral features? In the third example, we are motivated to develop a local representation of the microscopic dielectric response function of valence electrons.