Coupling between molecular excited states and plasmons in highly confined fields

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The coupling between molecular excited states are important for understanding single-molecules surface-enhanced Raman scattering, plasmon-exciton hybridization and energy transfer between molecules and metal nanoparticles. We will present our recent work on developing polarizable embedding models for describing molecules-plasmon interactions from first-principles. The focus will be on understanding the coupling of the molecular excited states with the plasmon excitation. We will discuss the importance of considering multiple excite states and molecular interactions for understanding plasmon-exciton hybridization.