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CCQ NYU
LIGHT-MATTER SEMINAR

Title: Effect of quantum and classical cavity model on the (molecular) polaritonic spectrum

Abstract: The quantum model of light employs Fock states, corresponding to different photon numbers, while in the classical model, the light is described by only two variables, corresponding to the photonic displacement field and the magnetic field, respectively. Both the quantum and the classical treatment of the cavity mode can explain the well known polariton splitting arising when the cavity frequency is resonant with a molecular transition. We are looking for phenomena, where the quantum and the classical treatment of the cavity leads to differences in the polaritonic spectrum. The test system is a single HCl molecule (which is always treated quantum mechanically), and we calculate the rotational-vibrational spectrum in the cavity. The spectrum is calculated from the eigenstates of the full cavity-molecule Hamiltonian in the case of the quantum cavity model, while the Fourier-transform of the dipole autocorrelation function is employed in the classical cavity model. In the quantum cavity case, if the cavity mode is in resonance with the “i -> f” rovibrational transition, we observe a polariton splitting not only for this transition, but also for other transitions whose final state is “f”, but these additional splittings are missing in the classical cavity model. This effect is seen for a simple 3-level model system, as well, and it is probably more general.