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Toward simulations of quantum dynamics at complex plasmonic interfaces

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Noble-metal nanostructures support collective electron resonances, known as plasmons, that can "squeeze" optical fields down to nanometer-scale volumes, well below the conventional diffraction limit. The strong localization of electromagnetic fields greatly enhances nonlinear optical processes, both in the metal nanostructure itself and in adjacent optical materials. Because the processes occur entirely within a sub-wavelength volume, the usual phase-matching conditions for these processes are lifted. Ensembles of quantum emitters optically coupled to plasmonic nanocavities, have recently emerged as new platforms for strong light-matter interactions. When the strength of coupling between the plasmons in the metal nanostructures and resonant materials (such as molecules, molecular aggregates, quantum dots) exceeds decay rates in the coupled system, new phenomena appear. In particular, mixed light-matter systems known as polaritons are formed in this "strong-coupling"regime. These quasiparticles synergistically combine the nonlinear properties of the plasmonic and excitonic constituents and are thus ideal for the development of efficient nonlinear photonic devices. As we advance our understanding of the physics of such systems the need for multiscale simulations arises. The major challenge is to combine Maxwell's equations with quantum dynamics pertaining to molecules driven by electromagnetic radiation, which results in a highly unbalanced load of multiple processors when done conventionally. In this talk I will discuss the efficient parallel methodology recently developed for simulating nonlinear dynamics of a large number of molecules with ro-vibrational degrees of freedom explicitly considered in time domain and directly coupled to Maxwell's equations in three dimensions in real time.

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