Properties of Molecular Exciton-Polaritons: Coupling *Ab Initio* Calculations with Quantum Optics

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Polaritonic chemistry has become the leading direction to control a multitude of processes, such as charge transfer, selective bond breaking, and excited state dynamics. An exciton-polariton is an entangled state of light and matter in which the native excitonic and photonic degrees of freedom hybridize to form new states. These new states can be tuned in various ways to modify and produce unique properties, such as the potential energy landscape or the emission efficiency of materials. However, much is still unknown about how these new hybrid states can modify such chemical properties. For example, the nature of the exciton is lost and becomes effectively mixed with all other molecular excitations, and so the shape and distribution of resulting exciton-polariton wavefunctions will be dramatically different from the uncoupled excitonic picture. These changes will dictate all the resulting properties, such as the absorption/emission spectra though the polaritonic transition dipole moments and the excited state dynamics through modification of the potential energy surfaces. In this work, we explore a set of real, atomistic molecules via time-dependent density functional theory and couple their electronic structure to a single-mode cavity in order to explore the resulting properties of the entangled light-matter system.