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Multiscale Modeling of Plasmon-Exciton Dynamics of Malachite Green Monolayers on Gold Nanoparticles[1] HOLDEN SMITH, Louisiana State Univ - Baton Rouge, TONY KARAM, California Instititute of Technology, LOUIS HABER, KENNETH LOPATA, Louisiana State Univ - Baton Rouge — A multiscale hybrid quantum/classical approach using classical electrodynamics and a collection of discrete twolevel quantum system is used to investigate the coupling dynamics of malachite green monolayers adsorbed to the surface of a spherical gold nanoparticle (NP). This method utilizes finite difference time domain (FDTD) to describe the plasmonic response of the NP and a two-level quantum description for the molecule via the Maxwell/Liouville equation. The molecular parameters are parameterized using CASPT2 for the energies and transition dipole moments, with the dephasing lifetime fit to experiment. This approach is suited to simulating thousands of molecules on the surface of a plasmonic NP. There is good agreement with experimental extinction measurements, predicting the plasmon and molecule depletions. Additionally, this model captures the polariton peaks overlapped with a Fano-type resonance profile observed in the experimental extinction measurements. This technique shows promise for modeling plasmon/molecule interactions in chemical sensing and light harvesting in multi-chromophore systems.

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