

Development and Application of the Hybrid Quantum-Classical Approaches for the Study of the Plasmon-Enhanced Molecular Spectroscopy

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Plasmonic MNPs, due to the dramatic effect of localized surface plasmon resonance (LSPR), have been widely used to control and manipulate light at the nanoscale, thus regulating the photophysical and photochemical behaviors of molecules in their vicinity. Because of the complex interplay between the plasmon and molecular quantum transitions, it is challenging to interpret the experimental phenomena and unveil the underlying interplay mechanisms. Computational simulation which bridges the gap between theory and experiment can reach such a goal. Many hybrid quantum-classical approaches have thus been developed to model the coupled plasmon-molecule systems. Here, I report our group's recent works on the study of plasmon-enhanced electronic and vibrational spectroscopy, especially focus on the implementation of the analytic high-order energy derivatives of (TD-)DFT/DIM into the electronic structure package to explore the MNP-mediated molecular potential energy surface and calculate molecular IR and Raman spectra.