Self-Consistent Modeling of Coupled Maxwell-Rate Equations with the Finite-Difference Time-Domain Method

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In this study, we introduce a semi-classical finite-difference time-domain (FDTD) framework for modeling molecule-plasmon interactions in three dimensions. By integrating molecular rate equations with electromagnetic field calculations on the Yee grid, the approach provides a self-consistent analysis of the dynamic coupling between molecular processes and plasmonic fields.

Introduction

The interaction between molecules and plasmonic nanoparticles is a cornerstone of modern nanophotonics, necessitating a rigorous description of both quantum molecular dynamics and classical electromagnetic fields. Existing methodologies often lack the capacity to resolve the temporal and spatial intricacies of these coupled systems. To address this challenge, we present a self-consistent semi-classical framework based on the finite-difference time-domain (FDTD) method. This approach integrates molecular rate equations directly within the electromagnetic field calculations, enabling detailed investigations of the dynamic coupling between molecular and plasmonic processes.

Results

The presented FDTD framework effectively captures the near-field and far-field optical responses of molecule-plasmon systems under various excitation conditions, including pulsed and continuous-wave inputs. Simulations reveal intricate energy exchange processes and elucidate the role of plasmonic fields in influencing molecular excitation and radiative emission dynamics. Numerical stability and accuracy are preserved across the spatial and temporal scales relevant to molecule-plasmon interactions. These results establish the framework as a robust computational tool for advancing the theoretical understanding and design of nanophotonic systems.

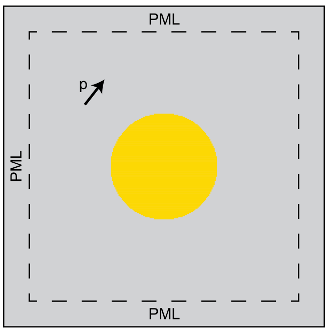

Fig. 1. 2D cross section of a molecule (dipole) and plasmonic (gold) nanoparticle 3D geometry.

References

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