Body-of-Revolution Finite-Element Model of Plasmon-Enhanced Fluorescence

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Plasmon-enhanced fluorescence (PEF) is one of the most widely investigated optical phenomena in hybrid systems of emitters and plasmonic nanoantennas, with applications ranging from biosensing to single-molecule emission microscopy. However, the computational optimisation of these systems is frequently hindered by the substantial memory and computational costs associated with full three-dimensional (3D) electromagnetic simulations. In this work, we extend finite-element modelling of PEF beyond spherically symmetric geometries using a body-of-revolution finite-element method (BOR-FEM). By exploiting exact or equivalent rotational symmetry, 3D emitter–nanoantenna systems are reduced to computationally efficient 2D formulations while retaining the essential electromagnetic interactions governing excitation and emission. We validate the framework against three previously investigated emitter–nanorod systems, including one requiring an equivalent axisymmetric geometric transformation, before applying it to an emitter–core–shell nanorod system. Specifically, we investigate the PEF of the terminal chlorophyll emitter of the major plant light-harvesting complex (LHCII), the most abundant membrane protein on Earth, interacting with a gold core-dielectric shell nanorod with one or two dielectric shells. The simulations reveal that the interplay between excitation enhancement, radiative-rate enhancement, and non-radiative Ohmic losses gives rise to four distinct shell-thickness-dependent operating regimes (quenching, enhancement, suppression, and decoupling), with recovery of the intrinsic quantum yield in the decoupling regime. The predicted enhancement factors for experimentally relevant dual-shell nanorods agree well with previously reported measurements. These results establish BOR-FEM as an efficient and versatile framework for modelling PEF in rotationally-symmetric nanoantenna geometries and in non-axisymmetric geometries that admit equivalent axisymmetric representations, providing a practical route for the rational design and optimisation of plasmon-enhanced bio-nanophotonic systems.

I. INTRODUCTION

Plasmon-enhanced fluorescence (PEF) arises from the modification of the excitation and emission processes of emitters placed in the near field of metallic or dielectric nanostructures. By tailoring the local density of optical states and restructuring the radiative decay channels, nearby nanoantennas can substantially enhance or suppress an emitter's far-field fluorescence intensity depending on the emitter–nanoantenna geometry, spectral overlap, and separation distance. The phenomenon can be traced back to the pioneering experimental and theoretical works of Drexhage on dipole emitters near dielectric interfaces [1, 2], followed by theoretical investigations of fluorescence modification near nanospheres [3, 4] and nanospheroids [5]. These foundational studies established the framework for what is now commonly referred to as *metal-enhanced fluorescence* (MEF) [6–8], or PEF [9–13]. Today, PEF constitutes a central topic in nano-optics and nanophotonics owing to its ability to control excitation rates, spontaneous emission rates through the Purcell effect, and nonradiative decay channels (emission suppression or quenching) [11, 12, 14, 15].

The ability of plasmonic nanoantennas to tailor light–matter interactions has enabled numerous technological applications. In photovoltaics, PEF has been used to modify the absorption and emission properties of solar cells, thereby improving their power conversion efficiency [16–18]. Similar concepts have been applied to light-emitting diodes, where plasmonic structures can increase emission efficiency and brightness [19, 20]. The strong electromagnetic hotspots associated with plasmonic resonances have also motivated the development of plasmon-enhanced microscopy techniques that offer improved image contrast and spatial resolution [21–23]. In biosensing, plasmonic enhancement has been used to provide enhanced detection sensitivity and signal-to-noise ratios, enabling applications ranging from point-of-care diagnostics and single-molecule detection [24–27] to real-time monitoring of binding kinetics [28, 29].

To understand and optimise these systems, extensive theoretical and computational studies have been devoted to calculating PEF in a wide variety of emitter–nanoantenna geometries. Representative examples include emitters near nanospheres [30, 31] and nanorods [10, 11, 14, 32–37], emitters in dimer nanoantenna gaps [32, 38–42], emitters inside [43, 44] and outside [10, 15, 45–47] nanoshells, and emitters near more complex nanostructures [48–51]. PEF has also been investigated in biohybrid systems involving photosynthetic light-harvesting complexes coupled to plasmonic nanoantennas [12, 52–54]. Quantitative modelling of these systems generally requires solving Maxwell's equations in three dimensions (3D) using numerical approaches such as the finite-difference time-domain (FDTD) method [12, 14], the boundary element method (BEM) [28, 29, 55], the multiple multipole method [14, 56], discrete dipole approximation (DDA) [11], and quasinormal modes analysis [57, 58].

For emitter–nanorod systems with rotational symmetry, the

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