Plasmon Enhanced Fluorescence Characteristics Government By Selecting the Right Objective Function

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Abstract

Core-shell type plasmonic nanoresonators have been optimized to maximize the fluorescence rate of coupled dipolar emitters, namely SiV color centers in diamond. The RF module of the COMSOL Multiphysics® software was applied to extract the optical response and to analyze the near-field and charge distribution. Conditional optimization has been performed by an in-house developed GLOBAL optimization algorithm. The criterion regarding deltaR radiative rate enhancement at the SiV excitation ensured that nanoresonators capable of enhancing excitation were evaluated, while the criterion regarding cQE corrected quantum efficiency at the SiV emission was modified in multiple steps. The optimization was performed by selecting either the product of the radiative rate enhancements at the excitation and emission nominated as Px factor, or the product of the Px*cQE as the objective function. Comparison of different coupled systems received via conditional optimization made it possible to uncover the advantages of different number of dipoles and types of nanoresonators, as well as of different optimization methods. To qualify the achievable fluorescence enhancements the Purcell factor, QE quantum efficiency and delteR radiative rate enhancement have been determined as function of wavelength. The quality factor of the optimized resonators was computed based on the extinction cross-section spectra extracted from plane wave illumination of nanoresonators of the specific geometry as well as based on the Purcell factor spectra.

Dependency of the two different FOMs on all geometrical parameters was inspected and compared for coupled systems optimized by applying the Px and Px*cQE objective functions. In addition to this the Px*cQE was inspected as a function of both composing quantities, while the Px was studied as a function of the cQE (Fig. 1). The achievable Px and Px*cQE quantities were compared for different number of dipoles, different types of nanoresonators and for different methods of optimizations. The comparative study revealed that all geometrical parameters are larger in core-shell type nanoresonators optimized with the Px*cQE objective function, since the larger dipole distance allows reaching larger cQE in larger nanoresonators.

The amount of accumulated charges is significantly smaller in case of nanoresonators optimized with the Px*cQE objective function, which reveals that the resonance is weaker, correspondingly the Purcell factor is smaller. Although, the quantum efficiency is considerably larger throughout the complete inspected spectral interval, the radiative rate enhancement is (larger) smaller at the excitation (emission) in case of nanoresonators

optimized by applying Px*cQE as the objective function. Accordingly, larger (smaller) lobes correspond to the nanoresonators determined by applying the Px*cQE objective function at the excitation (emission) wavelength. In accordance with the intuitive expectation, the Px (Px*cQE) is larger in systems optimized with the Px (Px*cQE) objective function.

The FWHM of the ECS and Purcell factor peaks are always larger, which implies that the quality factor is weaker in nanoresonators optimized to maximize for Px*cQE. This indicates that the main advantages of the optimization performed by applying the Px (Px*cQE) objective function manifest themselves in non-cooperative (cooperative) fluorescence enhancement.

Figures used in the abstract

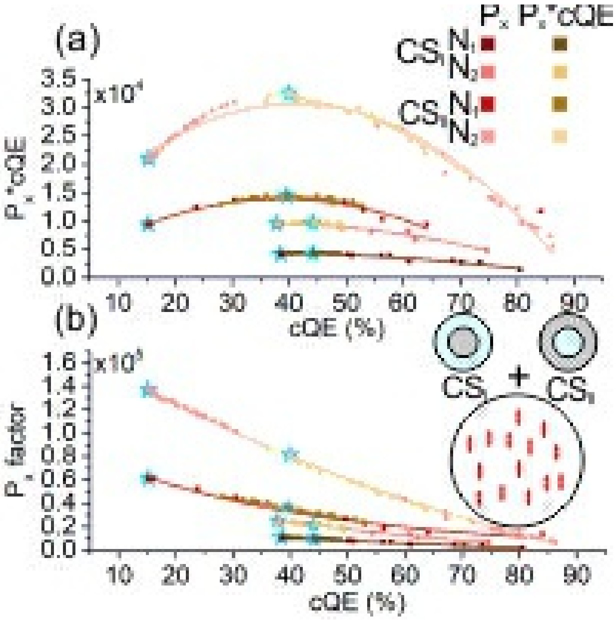

Figure 1: The Px*cQE and the Px FOMs as a function of cQE for different number of dipoles, types of nanoresonators and different objective functions.