Optimizing the Fluorescence of Diamond Color Centers Encapsulated Into Core-Shell Nano-Resonators

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Abstract

INTRODUCTION
Enhancement of a single-photon emission is a great demand in recent science and applications, including development novel class of light sources, encoded information transfer and biological imaging [1, 2, 3]. Fluorescence can be improved through excitation and emission enhancement. Improvement of these two processes can be realized by using the near-field enhancement accompanying the localized surface plasmon resonace (LSPR) nearby various metal nanoparticles. LSPR is a nanophotonical phenomenon, which results in a tight light confinement around conductive nanoparticles smaller than the wavelength of light. The characteristics of LSPR is strongly material and shape dependent [4]. In order to obtain the optimal geometric parameters of coupled plasmonic nanostructure - emitter system, numerical calculations are needed.

USE OF COMSOL MULTIPHYICS® SOFTWARE
Our purpose was to find the optimal configuration of a coupled core-shell - emitter system to enhance excitation or emission. We have modeled this nanophotonical problem in COMSOL Multiphysics® software using its RF Module. The emitter was placed into the center of a diamond nano-sphere and was modeled as an electric point dipole with a frequency of 532 nm excitation wavelength of nitrogen (NV) and silicon (SiV) vacancy centers, and of 650 nm and 738 nm emission wavelength of NV and SiV centers, respectively. The optical responses of the inspected configurations were determined by integrating the average power outflow through closed surfaces. The diamond core radius and gold shell thickness have been optimized by implementing the GLOBAL [5] algorithm using LiveLink™ for MATLAB®. The wavelength dependent properties of the optimized core-shell configurations have been determined by sweeping the dipoles wavelength in the interval of [400 nm, 900 nm] (Figure 1).

Two different approaches were compared, namely, setting a criterion to have a predetermined minimal quantum efficiency (QEcrit) of the configuration and maximizing the Purcell factor of the dipole, and the complement of this method (Pcrit).

RESULTS
The wavelength dependent Purcell factor (Purcell), quantum efficiency (QE) and the product of them (QExPurcell) qualify the excitation and emission enhancement. Therefore, these quantities of the optimal configurations obtained via both conditional optimization

approaches have been compared (Figure 2).

CONCLUSION
The maximum appearing on the spectra of the optical responses originates from the LSPR of the core-shell nanoparticles. Although, core-shell resonators exhibit single peak on their Purcell factors, tuning of these resonances to the excitation and emission wavelengths makes it possible to enhance both phenomena with good efficiency. The quantum efficiencies exhibit two local maxima besides the global maximum. The QE*Purcell product in the optimized systems shows a single peak, which is detuned from the excitation wavelength, while well approximates both of the emission wavelengths. The results of the two approaches compose theoretically the same set of optimal solutions, and each of these solutions are limited by the selected material and structure type. However, it depends on the starting criterion, which solution is found within the framework of analogous optimization procedures. These results show that requirement of specific applications determine, which quantity is better to optimize in the QE*Purcell product by setting a criterion on the other.

Reference

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Figures used in the abstract

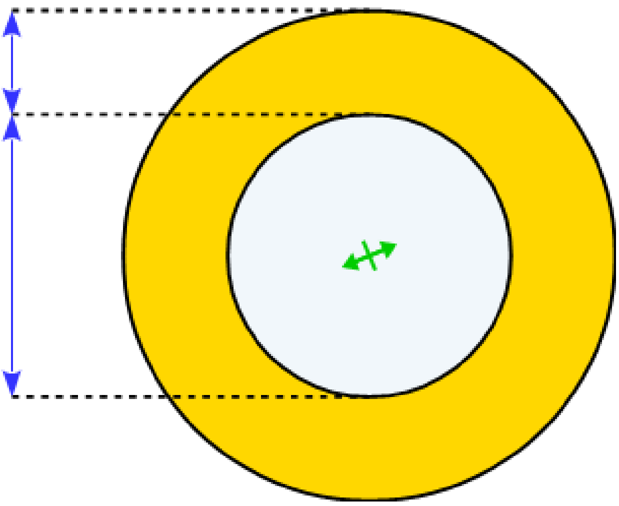

Figure 1: Schematics of the optimization methodology. Yellow: gold nanoshell; pale blue: diamond core; green arrow: oscillating dipole; blue arrows: core-shell geometrical parameter tuning.

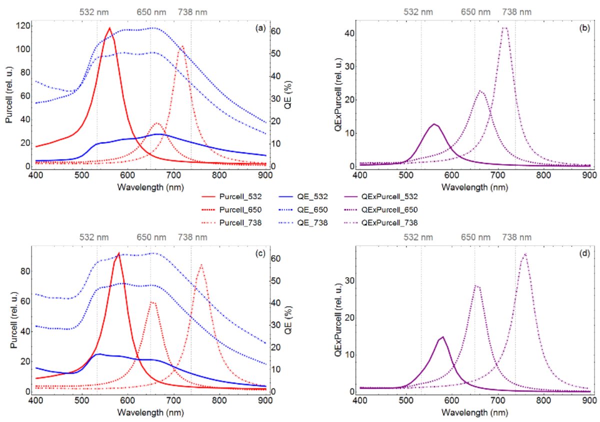

Figure 2: Wavelength-dependent optical response of the optimal configurations.