Photoluminescence spectral position shift governed by optical heating of perovskite resonant nanoparticles

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Abstract. Recent studies demonstrated high interest in halide perovskite materials for different applications including solar cells, light emitting diodes and many others. Moreover, it was revealed that resonant nanoantennas made of such materials can serve as efficient nanoscale light sources with tunable spectra in broad range by changing the composition of the initial perovskite material. However, resonant dielectric and semiconductor structure undergo considerable optical heating which affects the spectral position of the photoluminescence. In this paper we demonstrate theoretically photoluminescence shift for single resonant MAPbI$_3$ nanoparticle governed by temperature increase. Thus, our results can make resonant perovskite nanoparticles a promising platform for temperature-feedback optical heating and precise tuning of photoluminescence emission.

1. Introduction
Nanoscale light sources are basic elements for advanced nanophotonics application [1]. Among the most frequently used active light sources are nanoparticles with active defects [2] and quantum dot emitters [3]. But still, it remains a challenging problem to effectively steer and control the emission radiation pattern, even though various designs were introduced. Conventional methods of routing the emission often required multistage fabrication steps which resulted in sufficient increase of cost for practical implementations or placing nanoantennas near the active emitter, thus making the whole system non-robust against chemical pollution and mechanical damages.

On the other hand, it was revealed that nanoparticles made of organic-inorganic (hybrid) MAPb(I,Br)$_3$ perovskite materials can support Mie-resonance in the visible range, thus enhancing and guiding the photoluminescence (PL) emission from the nanoantennas [4]. Moreover, by selecting the initial perovskite compound, one can tune the PL spectra throughout whole visible range. However, even under moderate laser pump powers dielectric and semiconductor structures suffer from optical heating [5, 6], which affects spectral position of the PL peak [7].

In this work, we theoretically study PL spectral shift governed by optical heating of resonant MAPbI$_3$ nanoparticles. We believe that such approach can be promising for various applications, which require optical heating with fine tuning of emission spectrum, e.g. nanothermometry.
2. Results

In order to obtain deep understanding in optical heating of perovskite spherical nanoparticles, theoretical calculations should be applied. It was shown that the absorbed power $P_{abs}$ by the nanoparticle is proportional not only to conductivity $\sigma$ of the material, but also to the field enhancement factor $F$ inside the nanostructure [5]. Thus:

$$P_{abs} = \int J^* E dV \sim \sigma E^2 F,$$

(1)

where $J$ is optically induced current in the nanoparticle, $E$ electric field. It means that efficiency of conversion of incident light to thermal heat energy is strongly dependent on resonant behaviour of the nanostructure. Indeed, temperature increase of the nanoparticle under CW illumination in homogeneous media can be found by following expression [8]:

$$\Delta T = \frac{IC_{abs}}{4\pi \kappa R},$$

(2)

where, $I$ intensity of the incident light, $C_{abs}$ absorption cross section, $\kappa$ thermal conductivity of the surrounding media and $R$ radius of the spherical nanoparticles.

Figure 1 demonstrates optical heating of a single spherical nanoparticle in homogeneous air media for different real and imaginary parts of permittivity for fixed wavelength over diameter ratio $\lambda/D = 1.95$. Blue dots represent dispersion of the materials at incident wavelength of 633 nm, thus making perovskite nanoparticles of MAPbI$_3$ compound a better structure for efficient optical heating than crystalline silicon for given conditions. However, heating of the perovskite affects the optical properties of its PL emission. Indeed, Figure 2(a) shows experimental results on shifting of the bulk MAPbI$_3$ PL peak spectral position with increase of the temperature [7]. With higher temperatures PL spectrum undergoes blue-shift. Figure 2(b) shows theoretical calculations on PL peak spectral position governed by optical heating of the...
resonant MAPbI₃ nanoparticle. The general tendency of stronger blue shift with the increase of the size is reasonable due to Eq. 2, where absorption cross-section increases with the second power of the size parameter (radius), whereas in the denominator radius appears in the first power, thus for non-resonant spherical structures heating grows linearly with size. However, if we study resonant nanoparticle one can see resonant behaviour in the PL peak shift, which occurs due to excited optical electric and magnetic modes, thus enhancing absorption of light. Mode decomposition for different sizes of MAPbI₃ nanoparticles reveals magnetic dipole (MD) resonance with approximately 110 nm radius, mixture of electric dipole (ED) and magnetic quadrupole (MQ) with 160 nm and electric quadrupole (EQ) with 210 nm radius at a wavelength $\lambda$ of 633 nm.

3. Conclusions
In summary, we have theoretically demonstrated the ability for optical heating of resonant MAPbI₃ nanoparticles with possibility of precise tuning of their PL emission spectra, thus making such structures a promising platform for optical nanothermometry and thermo-optical detectors.

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Figure 2. (a) Experimental dependence of photoluminescence spectral position on temperature for MAPbI₃ [7]. (b) Theoretical photoluminescence spectral position dependence of a single spherical nanoparticle on radius, which undergoes optical heating by HeNe laser ($\lambda$=633 nm) with intensity of 0.05 mW/µm².
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