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### Bound-state in the continuum of a photonic crystal metasurface: a platform for ultrasensitive sensing and near field amplification

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Abstract. The localization of the electromagnetic field at the nanoscale can play a key role in many applications, such as sensing, spectroscopy and energy conversion. In the last years, great efforts have been performed to study and realize all-dielectric loss-free nanostructures to confine the radiation without the limits imposed by the plasmonic systems. Here we demonstrate that the field enhancement in proximity of a photonic crystal metasurface supporting bound states in the continuum can be explored to boost the light-matter interaction. We design and realize an innovative sensing scheme for bulk and surface measurement with ultra-high figure of merit and apply this new configuration for studying a specific protein-protein interaction. The recognition scheme can be coupled to a fluorescence-based sensing approach, which exploits the capability of the sensor to strongly enhance fluorescence signals. Our results provide new solutions for light manipulation at the nanoscale, especially for sensing and nonlinear optics applications.

#### 1. Introduction

Optical biosensors are widely-used devices that offer great advantages over conventional detection techniques in many crucial applications from health-care and food quality control to environmental analysis and industrial process monitoring [1-4]. A widespread class of label-free photonic biosensors exploits optical resonance effects where the shift in the resonance wavelength in response to a change of the refractive index (RI) of the medium surrounding the sensing area gives information about the analyte. Based on this mechanism, surface plasmon resonance (SPR) and localized SPR (LSPR) devices are widely employed and are typically characterized by high values of sensitivity (S =  $\Delta RI/\Delta\lambda$ ) [5-6]. However, the large plasmonic optical losses, leading to resonance broadening, strongly affect their main figure of merit (FOM), commonly defined as the ratio between the sensitivity and the resonant peak width. In addition, these high optical losses induce local heating that can cause damages to the biological material under investigation and to the nanostructure itself by altering its photonic properties. For this reason, great efforts have been made to overcome the limits of the conventional plasmonic devices, taking advantage of near-field enhancement in loss-free dielectric material [7-10]. It has been demonstrated that an all-dielectric photonic crystal metasurface (PhCM) can support Bound States in Continuum (BIC), resonant states of infinite lifetime, experimentally involving very narrow coupled resonances, with a high Q-factor and a possible extremely large field intensity enhancement, up to 6 orders of magnitude larger than the intensity of the incident beam [11-16]. Herein, the design and realization of an innovative sensing platform for bulk and surface measurement is reported. The device exploits a normal-to-the-surface optical launching scheme to easily excite high Q-factor resonances

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associated with BICs supported by the PhCM. The sensing performances of the device and the capability of the metasurface resonance, showing a large near-field amplification, to sense the perturbation of the dielectric environment have been characterized. In addition, the ultra-high figure of merit of the device enables the recognition of protein-protein interaction and the detection of low molecular weight molecules. Finally, we observe a significant amplification of the fluorescence emission and Raman scattering of probe molecules on the same nanostructures, crucial point for label-free spectroscopic imaging in biomedicine.

#### **Results and discussion**

The samples are realized in silicon nitride  $(Si_3N_4)$  deposited by plasma-enhanced chemical vapor deposition (1%SiH<sub>4</sub>/Ar 100 sccm and N<sub>2</sub> 50 sccm) on a SiO<sub>2</sub> substrate. The PhCM structure consists of cylindrical air holes arranged in a square lattice and patterned in the silicon nitride film by means of electron beam lithography, transferred by coupled plasma etching process using CHF<sub>3</sub> and O<sub>2</sub> (Figure 1(a)). The lattice parameters (hole radius and depth and lattice constant) are optimized in order to excite the BIC resonance at around 760 nm. Numerical simulations show that the BIC mode behaves as an evanescent surface wave that cannot couple to free-space modes. The electromagnetic field is mostly confined at the interface between the photonic crystal and the quartz substrate, but the field enhancement at the PhC/Air interface was supposed high enough to provide a strong light–matter interaction over the surface [17].

A microfluidic chamber in PDMS (polydimethylsiloxane), consisting of a circular chamber with a diameter of 2 mm, was integrated with the PhCM. A sketch of the final device is shown in Fig. 1(b). The liquid flow was controlled by means of a syringe infusion pump (KD Scientific), allowing the control of the total infusion volume. In order to test the sensing capability of the PhCM device, Isopropyl alcohol/water solutions with different concentration were infiltrated in the chamber. Transmission spectra were acquired from the sample illuminated by a normally incident supercontinuum laser (NKT Photonics) by means of an Ocean Optics USB4000 spectrometer with a resolution of 0.25 nm. The results are shown in Figure 1(c). When the RI changed from 1.3437 to 1.3652, the whole transmission spectrum shifted toward the red. By monitoring the peak of the spectrum as a function of the solution RI, the sensitivity curve was reconstructed. The linear fit of the experimental curve revealed a bulk sensitivity  $S = \Delta \lambda / \Delta n = 237.1 \pm 14.7 \text{ nm} / RIU$ . Remarkably, this value was found to be independent from the incidence angle of interrogation, demonstrating that no particular care had to be taken to align the beam along the normal incidence [18]. This feature is consistent with the properties of a resonance-trapped BIC for which the Q-factor remains large even far from the high symmetric  $\Gamma$ point [19] and represents am advantage for real-world applications. In addition, taking into account the sharpness of the resonance, a FOM up to 445 of our BIC-based sensor can be estimated [18]. This allows to appreciate variations of the order of the instrumental spectral resolution, enabling the detection of low molecular weight molecules, a significant advantage of the BIC mode with respect to the LSPR in metal sensors [18], [20].

The same sensing mechanism was applied also to the study of a specific biological problem, the recognition of a protein-protein interaction, i.e. detecting the association between the interacting domain of p53 and its protein regulatory partner murine double minute 2 (MDM2) [17], [21-22]. The method can be extended to the study of the dissociation effect exerted by other molecules, even at the nM range, therefore being of great importance in the first approach towards the discovery of substances with pharmacological activity against cancer.

The extremely high electromagnetic field enhancement and confinement on the dielectric metasurface by exciting the distributed optical resonance related to the BIC can be also used to achieve concurrent enhancements of  $\sim 10^3$  fold of fluorescence emission and Raman scattering far-field intensities of molecules dispersed on these metasurfaces [23].

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**Refractive index** 

Figure 1: (a) Scanning electron microscopy image of the photonic crystal (PhC) sample. The design consists of air-cylindrical holes arranged in a square lattice (a = 521 nm, r = 130 nm, h = 78 nm). (b) Sketch of the device: a PDMS microfluidic chamber was bonded to the PhCM. The inlet and outlet allow the controlled injection of the fluid. (c) Reconstructed sensitivity curve; the linear fit (orange curve) to the experimental data (black dots) revealed a bulk sensitivity S=237 nm/RIU.

#### 2. Conclusions

In this work, the realization of a new label-free resonant optical biosensor overcoming the limits of the classical plasmonic configurations has been proposed. The device is based on a PhCM nanostructure supporting a collective resonant effect due to the presence of bound states in the continuum. The sensor platform is characterized by a good sensitivity of 237 nm/RIU and a FOM as high as 445, which enables detection limits surpassing that of standard plasmonic sensors. The interrogation scheme requires minimal far field optical equipment, and is extremely robust to optical misalignment. In addition, the sensing configuration is highly versatile, as it can be optimized to work in a wide wavelength range, and its operation is free from interference of multiple modes. This all-dielectric platform can be explored

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also to boost the fluorescence emission of probe molecules of  $\sim 10^3$ -fold with a beam waist of solely 1.5 µm. Because of its unique characteristics, the novel device can be used both in label-free and fluorescence-based sensing configurations, with perspective performance and characteristics beyond the ones of technologies nowadays considered gold standards in the biosensing field. The behaviour of the sensor device in different ranges of refractive index is under investigation.

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