Anapole modes enabling linear and nonlinear chiral sensing in hybrid metasurfaces

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Abstract: In this work, we present how anapole modes can be exploited in hybrid metasurfaces to significantly enhance circular dichroism (CD) up to 5 times. Our results demonstrate that this metasurface offers efficient generation of background-free nonlinear CD signals, up to a 10-fold enhancement, that complements linear CD measurements.

Chirality, denoting the lack of specular symmetry in any plane of an object and the resulting existence of two mirror images (enantiomers), is a key aspect for the understanding of the biological functionality of many molecules in the human body and pharmaceutical compounds [1]. This recognition has sparked a growing industrial interest in discriminating molecular chirality, given its implications for drug efficacy and safety.

One of the key challenges in finding new ways to enhance the intrinsically weak circular dichroism (CD) chiroptical effect, thus enabling an efficient chiral sensing. Over the past decade, the design and development of nanophotonic platforms tailored for this purpose have emerged as a significant area of research and innovation. Fundamentally, the CD effect is proportional to the local Optical Chirality Density (OCD) C [2], defined as

$$C = -\frac{\omega\varepsilon_0}{2}\Im(\mathbf{E}^* \cdot \mathbf{B}) = -\frac{\omega}{2c^2}|\mathbf{E}||\mathbf{H}|\cos(\Phi)$$
(1)

where ω is the angular frequency, *c* the speed of light, ε_0 is the vacuum electric permittivity and Φ is the phase angle between *iE* and *H*. In the case of plane waves in vacuum Φ is maximized when the polarization is circular. The overall nanophotonic enhancement of the CD effect comes from the ratio between the spatial average of this quantity over the sample volume and the OCD of circular light.

As can be seen in equation 1, OCD enhancement at a particular wavelength can be achieved by local field concentration in nanophotonic structures while the phase relation $\cos(\Phi)$ is preserved. Various approaches have been explored to address this challenge. For instance, proposals based on plasmonics have exploited the substantial electric field enhancement generated by Surface Plasmon Resonance (SPR) [3]. On the other hand, the use of High Refractive Index Dielectric (HRID) materials has gained attention due to their low-loss nature and mixed electric and magnetic resonances, which can enhance both fields [4]. Hybrid structures, combining synergistically metallic and dielectric features, have emerged as particularly promising candidates [5].

In particular, HRID structures exhibit the noteworthy capability to sustain anapole resonances, characterized by intense optical field confinement. In the context of chiral sensing, this feature is interesting for background-free OCD enhancement as the phase relation of circularly polarized light is preserved [6]. Complementarily, this field confinement in anapole resonances can be exploited to enhance nonlinear optical effects, notably Third Harmonic Generation (THG). For example, HRID materials, with high third-order susceptibilities, have been combined with metallic materials to enable highly efficient THG in hybrid systems [7].

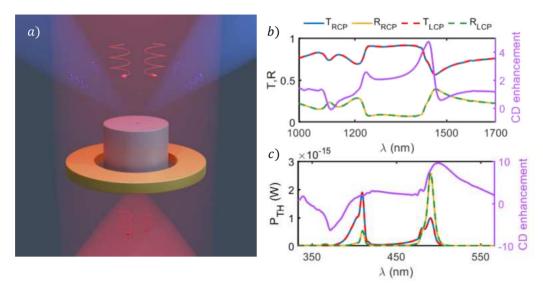


Figure 1. a) Depiction of the unit cell of the proposed metasurface. b) Linear reflectance and transmittance results of the proposed metasurface, together with linear CD enhancement up to 5 times. c) Third Harmonic Generation from the metasurface (reflection and transmission directions), with its associated CD signal, reaching a 10-fold enhancement at 490 nm.

In this study, we demonstrate numerically the efficacy of a hybrid structure (Figure 1a) consisting of a HRID (amorphous silicon) slotted nanodisk coupled to a gold ring as a promising platform for chiral sensing. This configuration yields a broadband, high average OCD value throughout a significant volume due to the confinement of electric and magnetic energy near anapole resonances. Additionally, we leverage these resonances to achieve a background-free, enhanced nonlinear third harmonic CD signal, with theoretical efficiencies up to 0.08%. Our results, summarized in Figure 1, show that CD enhancement can be 5-fold in the linear regime (Figure 1b) and up to 10 times in the third harmonic regime (Figure 1c).

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