Ultrathin WSe2 Metasurfaces For Efficient Nonlinear Nanophotonics: A COMSOL Multiphysics Study

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Abstract

1.Introduction
In on-chip nonlinear optical devices, a critical challenge lies in achieving high-efficiency second-order nonlinear processes, such as second-harmonic generation (SHG), in ultrathin materials, which essential for development of efficient modern nanophotonics. Transition metal dichalcogenides (TMDs) like WSe2 offer promising optical nonlinearities due to their broken inversion symmetry in monolayer form, but their nanometric thickness limits conversion efficiencies. Bulk WSe2, while centrosymmetric, can be engineered into metasurfaces to exploit quasi-bound states in the continuum (q-BICs) for field enhancement. While using thicker, multilayer WSe2 could increase the interaction volume, the common and most stable 2H crystal phase is centrosymmetric, which forbids second-order nonlinear effects in the bulk. However, fabrication imperfections, such as edge roughness, introduce scattering losses that degrade high-Q resonances essential for boosting SHG.

2.Device structure
The device structure consists of an ultrathin WSe2 flake with a thickness of 0.7 nm placed on a transparent glass substrate. The flake is patterned into a square lattice with a pitch of approximately 500 nm, where each unit cell contains a nanohole. Initially defined as circular holes with diameters of 300 nm, the features are transformed into equilateral triangular holes with side lengths of 375 nm. This geometry provides broken in-plane symmetry while maintaining subwavelength dimensions, enabling strong optical confinement and efficient nonlinear response.

3.Results
This work addresses the problem by designing and simulating ultrathin WSe2 metasurfaces with atomically precise triangular edges, achieved via anisotropic wet etching of pre-patterned circular holes, to break in-plane symmetry and enable q-BIC resonances for over three orders of magnitude SHG enhancement.
Two metasurface designs are investigated: Figure1: (i) circular nanohole arrays with C_4 in-plane symmetry, and (ii) triangular nanohole arrays produced by breaking C_2/C_4 symmetry. Simulation results reveal that while circular holes support symmetry-protected BICs that are challenging to excite from the far field, triangular arrays enable direct coupling to q-BIC resonances under normal incidence. Optimized triangular WSe_2 metasurfaces with a thickness of 0.7 nm, pitch of ~500 nm, and triangular side lengths of 375nm demonstrate SHG enhancements exceeding three orders of magnitude compared to bare flakes. The peak nonlinear conversion efficiency approaches 10^{-3} at pump wavelengths in the 800-850 nm range, in close agreement with reported experimental values for TMD-based metasurfaces. Furthermore, the triangular geometry yields cleaner resonances and reduced scattering losses due to sharper edges, as confirmed by near-field distribution plots and quality factor analysis within COMSOL.
We utilized COMSOL Multiphysics® software to model and optimize the metasurface design. The problem was set up using the Wave Optics Module within COMSOL Multiphysics® version 6.3. A 2D periodic unit cell geometry was created to represent the square lattice of triangular holes in WSe2 on a glass substrate, with parameters including lattice pitch (Λ = 500 nm), hole side length (atri = 375 nm), and flake thickness (h = 0.7 nm). The Electromagnetic Waves, Frequency Domain interface simulated light propagation, incorporating WSe2's anisotropic refractive index (n > 4) and second-order susceptibility χ2 (~10-10 m/V) from literature data. Boundary conditions included Floquet periodicity for the lattice and perfectly matched layers to mimic infinite extent. We solved for reflection spectra and electric field distributions at pump wavelengths (800-1050 nm) to identify q-BIC modes around 1.5 eV.
Simulations predicted SHG enhancements up to 1500-fold at resonant wavelengths (~810 nm), with q-BIC modes showing quality factors >1000, compared to bare WSe2 flakes. Obtained results matched experimental trends, validating edge sharpness in reducing losses.

4.Conclusion
In conclusion, these findings highlight the capability of COMSOL Multiphysics® to model and optimize ultrathin nonlinear metasurfaces, providing predictive insights into geometry-dependent SHG enhancement. The results indicate that WSe_2, with its strong χ2 response and high refractive index, is a highly attractive platform for realizing compact frequency converters, electro-optical modulators, and integrated quantum photonic devices. In future work, the models will be extended to investigate active tuning of SHG via electrostatic gating, strain engineering, and hybrid coupling with localized quantum emitters.

Reference

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Figures used in the abstract

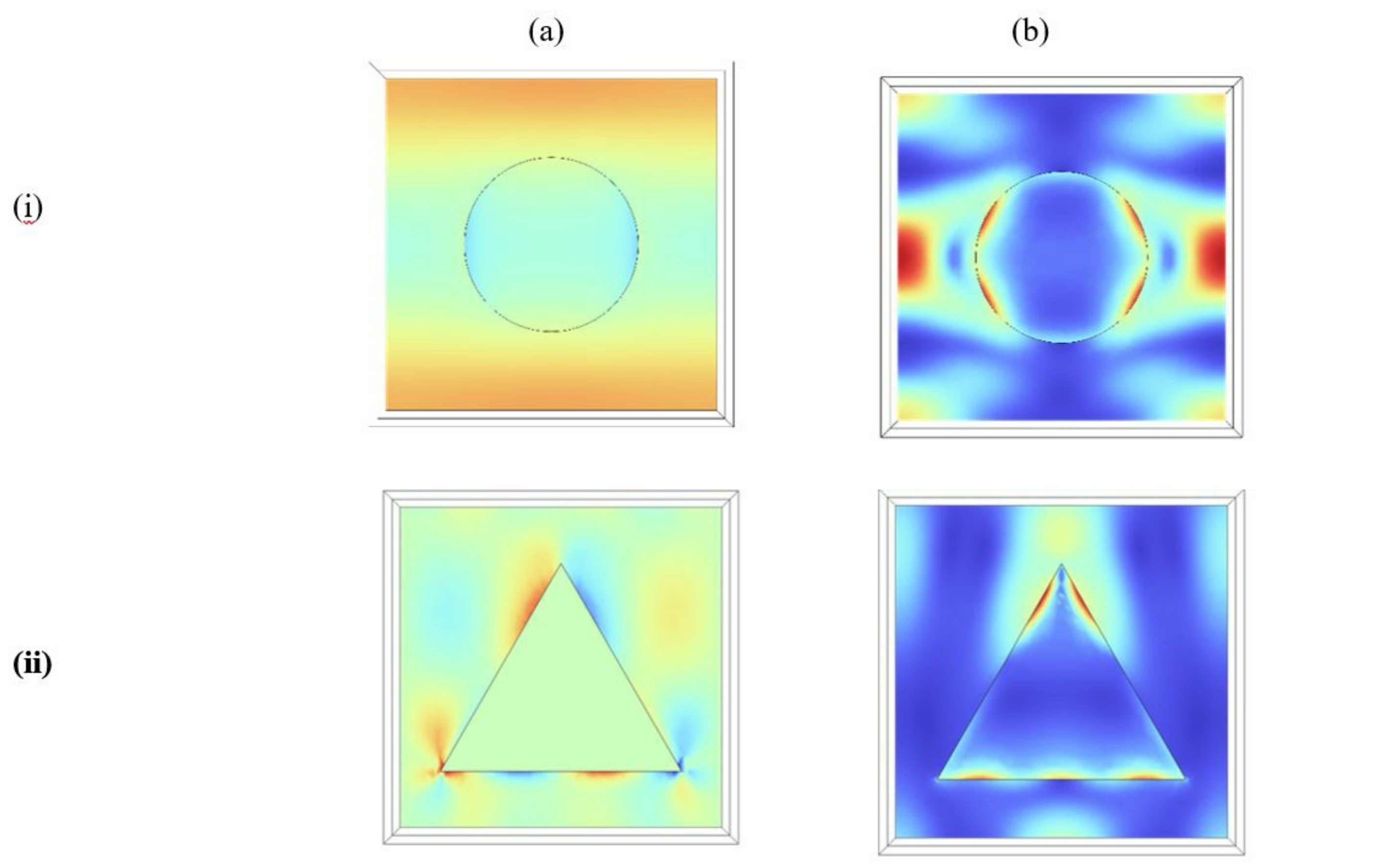

Figure 1 : (i) Circular nanohole arrays (ii) triangular nanohole arrays (a) First Electromagnetic Waves (b) Second Electromagnetic Waves

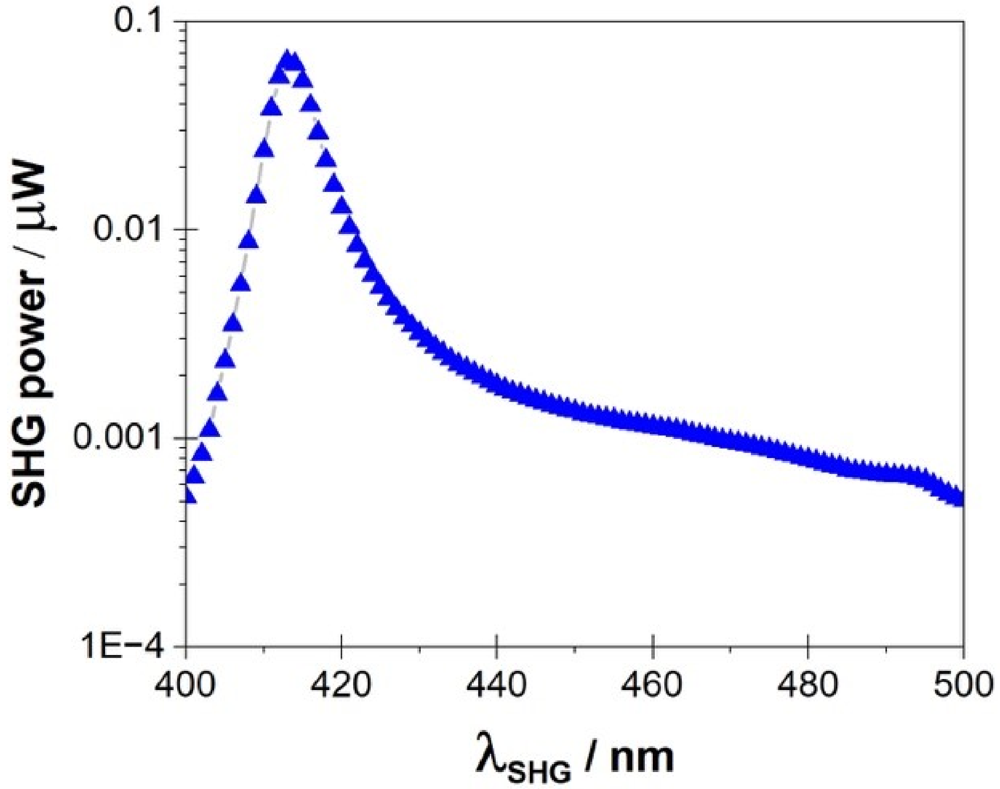

Figure 2 : SHG spectrum of triangular nanohole arrays showing a maximum second-harmonic intensity