Legume: A guided-mode expansion method for photonic crystal slabs for inverse design and light-matter interaction

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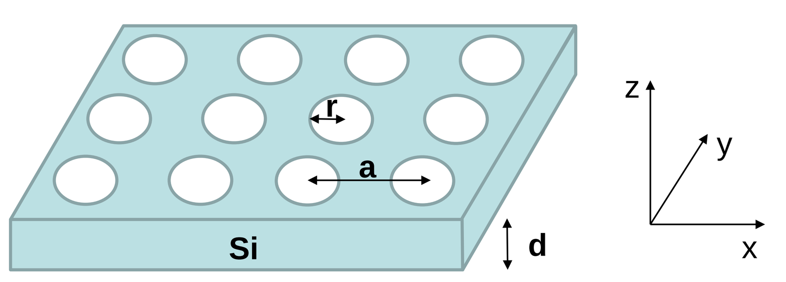
Introduction

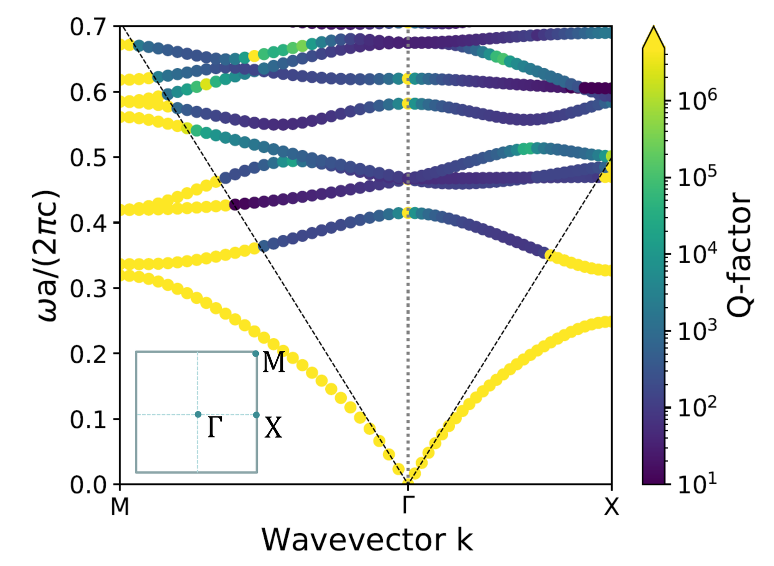
Photonic crystals (PhCs) embedded in slab waveguides, also known as PhC slabs, support truly guided and quasi-guided photonic modes [1]. PhC slabs lend themselves to the design of linear waveguides and nanocavities, the latter supporting fully confined cavity modes with low mode volumes and ultra-high Q-factors. Applications of PhC slabs can be empowered by inverse design techniques.

Here we present `legume`, a free python implementation of the Guided-Mode Expansion (GME) method for calculating photonic mode dispersion and losses in PhC slabs [2-5]. `legume` can be used for inverse design [3], as it embodies the Autograd backend for automatic differentiation. It can treat active two-dimensional layers with an excitonic resonance, allowing to describe the strong-coupling regime leading to photonic crystal polaritons [4].

Guided-Mode Expansion and legume

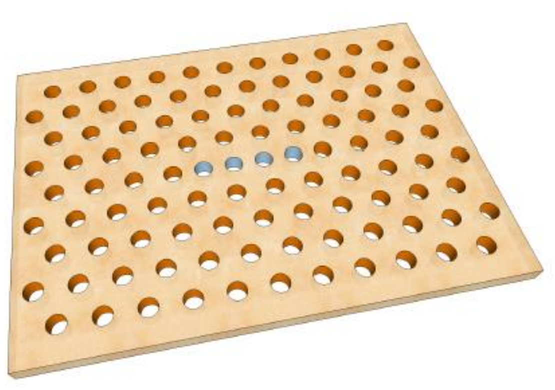
PhC slabs combine the features of 2D photonic crystals and of slab waveguides. In the GME method, the e.m. field is represented as a combination of 2D plane waves in the xy plane and guided modes along z. For quasi-guided modes that fall above the light line of the cladding material(s), diffraction losses are calculated by photonic perturbation theory.

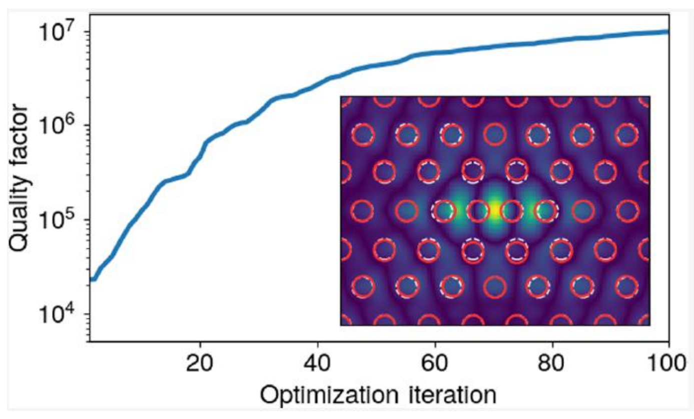




Photonic bands and Q-factors of a square-lattice photonic crystal slab in a silicon membrane ($n = 3.48$, $d = 0.3a$, $r = 0.3a$). Notice the appearance of infinite-Q modes above the light line (*bound states in the continuum*) at $k = 0$ and $k \neq 0$.

In the `legume` implementation of GME, inverse design can be performed by activating the interface to Autograd and using common gradient-based methods for minimization.





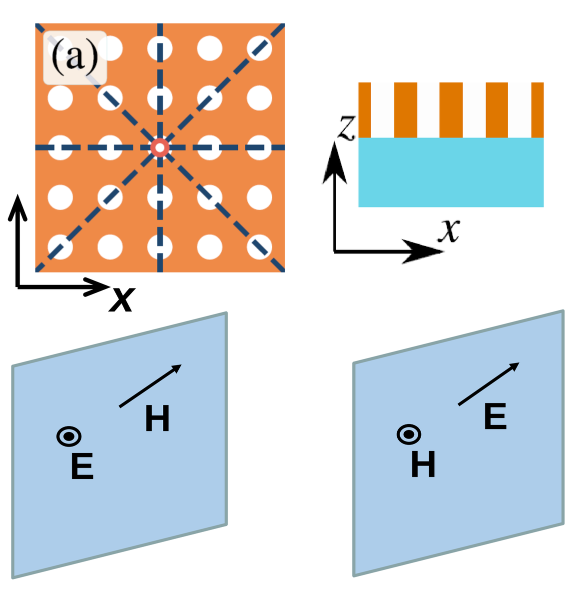
This example [3] shows the optimization of an L4/3 cavity in Lithium Niobate (n=2.21) with respect to the positions of nearby holes → 70 free parameters

Starting cavity: $Q \sim 6000, V = 0.61 \left(\frac{\lambda}{n}\right)^3$ After optimization: $Q \sim 0.97 \cdot 10^7$, $V = 0.49 \left(\frac{\lambda}{n}\right)^3$

The new version of legume [4] implements two key features: (i) symmetrization with respect to a vertical mirror plane, and (ii) interaction of photonic modes with 2D excitons, in order to describe the strong-coupling regime leading to photonic-crystal polaritons.

Symmetry and polarization mixing

We give an example of symmetry separation with respect to a vertical mirror plane, and comparison with Rigorous Coupled-Wave Analysis (RCWA).



s-pol, $\sigma_{kz} = -1$ (vertically odd)

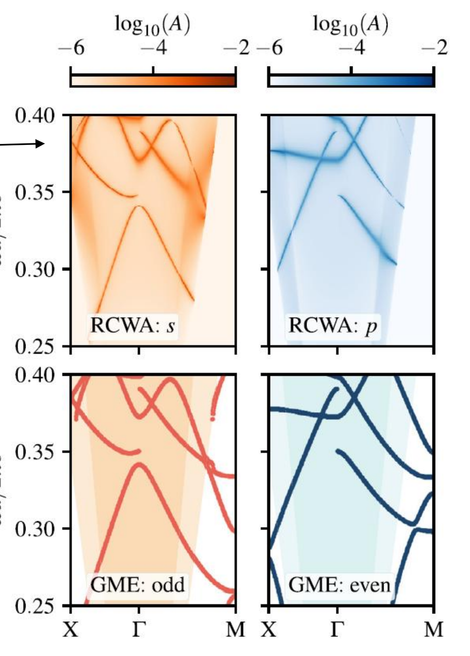
p-pol, $\sigma_{kz} = +1$ (vertically even)

RCWA absorption (with $\Im(\varepsilon_{GaAs}) = 10^{-4}$)

Vertically odd ($\sigma_{kz} = -1$) photonic modes are probed by s-polarized light

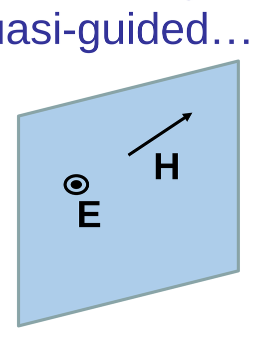
Vertically even ($\sigma_{kz} = +1$) photonic modes are probed by p-polarized light

Question: can s-polarized modes couple to p-polarized light in the far field, and vice-versa? i.e., *can polarization mixing occur*?

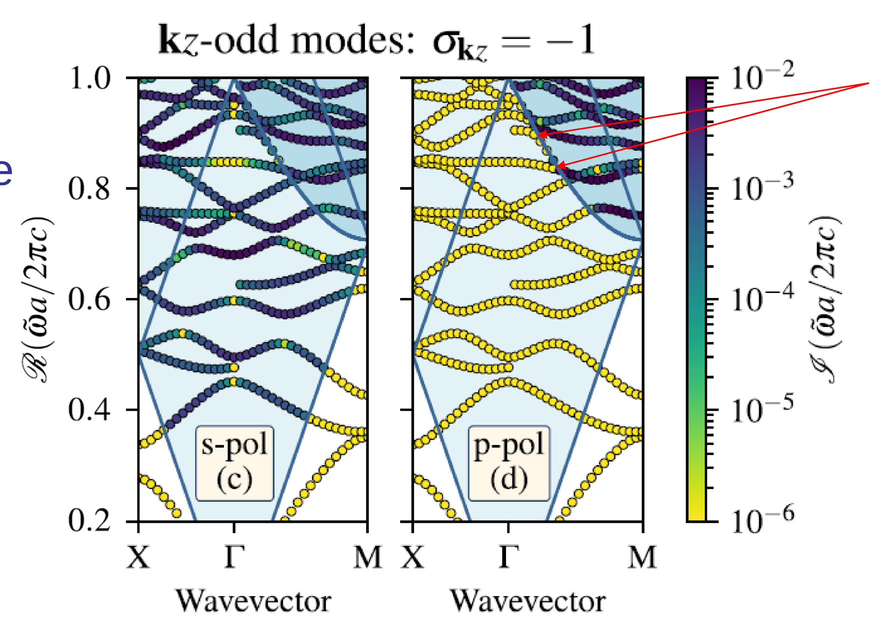


Parameters: square lattice with period a, slab thickness $d/a = 0.5$, hole radius $r/a = 0.2$, slab index $n = 3.54$, glass index $n = 1.45$

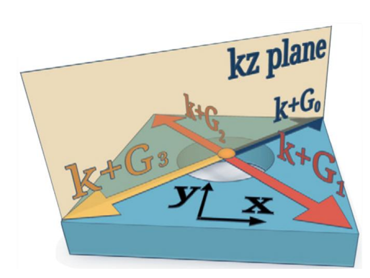
Vertically odd modes are coupled to s-polarized far field above the air light line, i.e., as soon as they become quasi-guided…



s-pol, $\sigma_{kz} = -1$ (vertically odd)



… but they are also coupled to p-polarized far field, above the cutoff for diffraction out of the plane of incidence

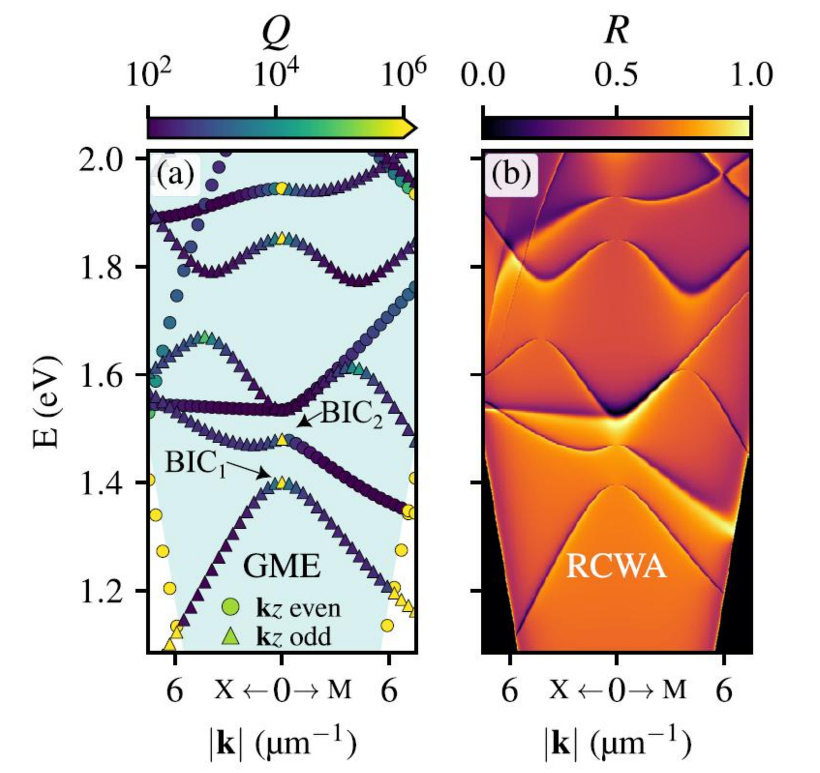


Polarization mixing can occur above the cutoff for out-of-plane diffraction.

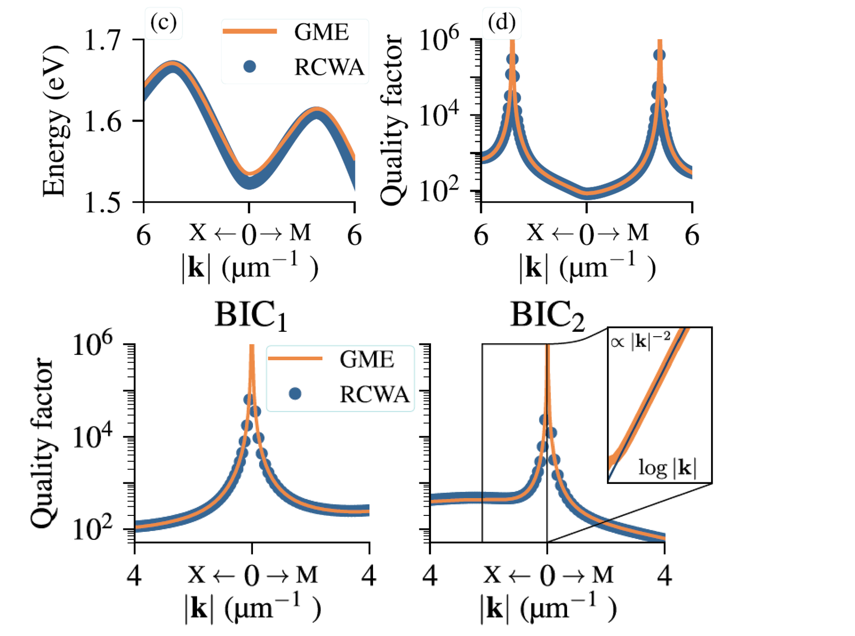
Bound States in the Continuum

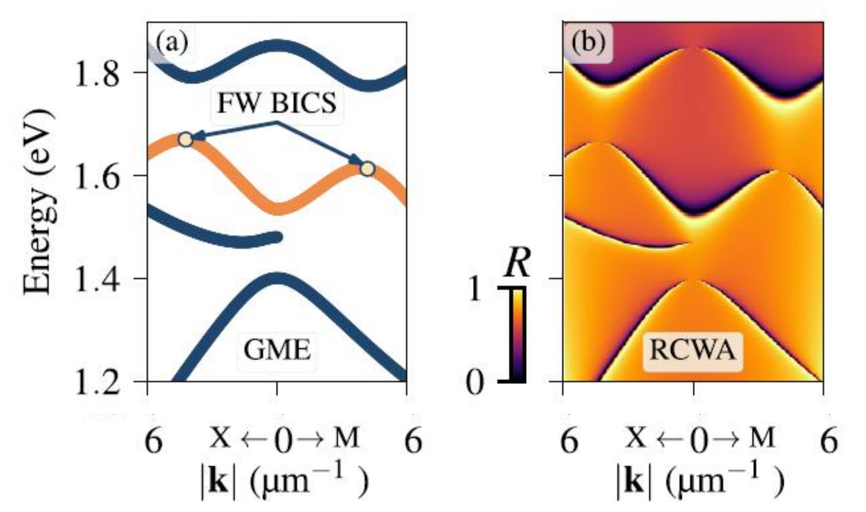
BICs are solutions of the wave equation that lie in the region of the continuous spectrum, but are uncoupled to the continuum. They can be of various kinds: symmetry-protected, Friedrich-Wingten if related to anticrossing, accidental.

Symmetry-protected and Friedrich-Wintgen BICs: comparison with RCWA

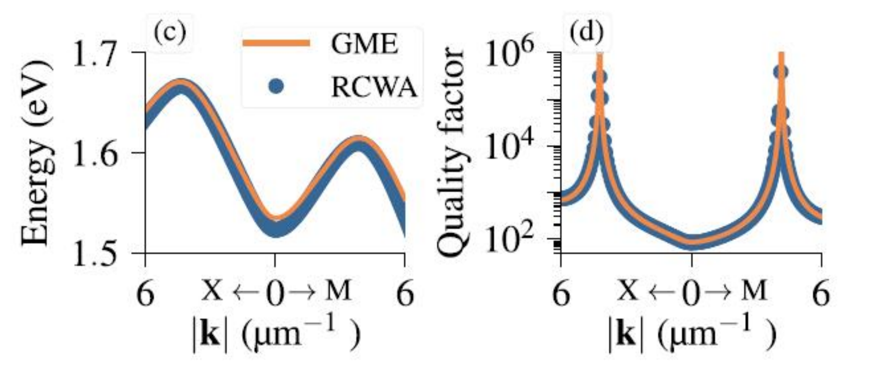


For a symmetry-protected BIC, $Q \propto \alpha^{-2}$, where α is the symmetry-breaking parameter [6]. Close to $k = 0$, we have $Q \propto k^{-2}$.





Use of symmetry with respect to a vertical mirror plane (**k**z-odd modes) to identify Friedrich-Wintgen BICs.



Photonic Crystal Polaritons

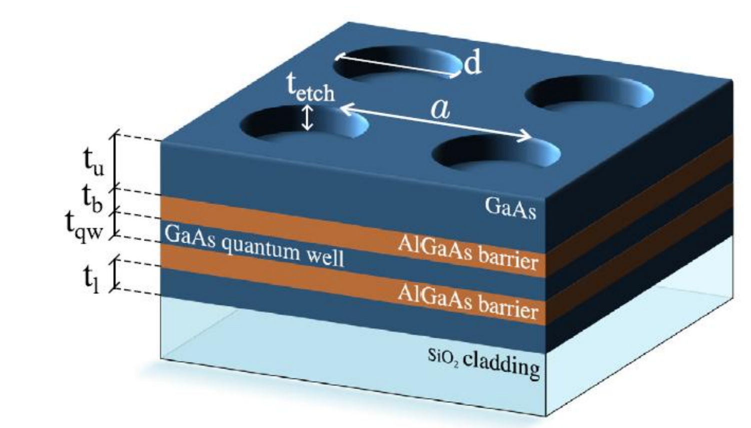
Polaritons are mixed modes of the electromagnetic field coupled to a material excitation: they are half light, half matter. 2D polaritons can be realized by coupling 2D photons (in a microcavity, or in a PhC slab) with 2D excitons in quantum wells.

We implement a quantum theory of photonic crystal polaritons. The PhC slab contains active layers, which support an excitonic resonance characterized by a resonance frequency, a linewidth, and an oscillator strength per unit area. The full Hamiltonian describing photons, excitons, and their mutual interaction is written in second quantization and diagonalized exactly by a Hopfield transformation [7-9]. The basis of photonic modes is the same of the Guided-Mode Expansion.

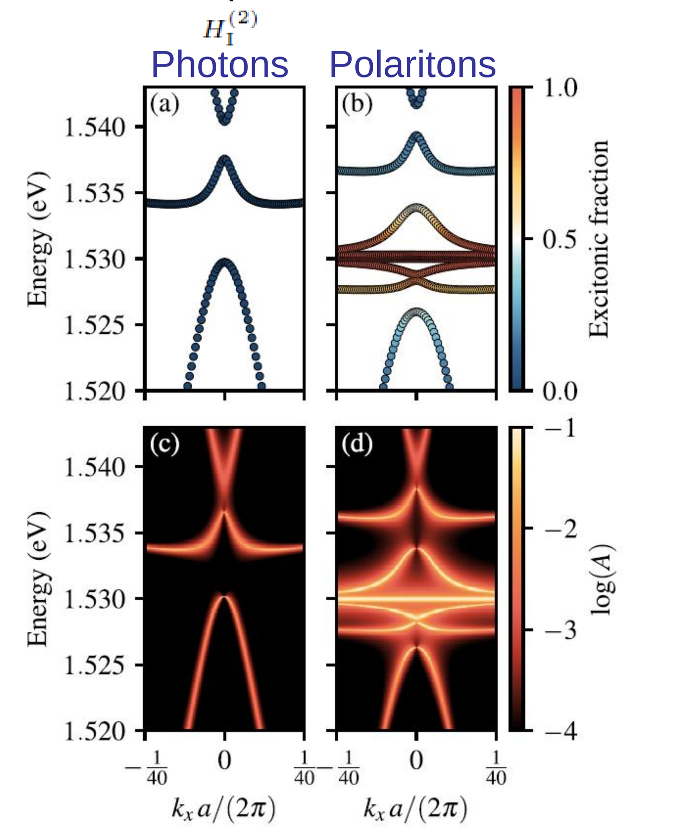
$$H_{\mathbf{k}} = \underbrace{\sum_n \hbar\omega_{\mathbf{k}n}\hat{a}^\dagger_{\mathbf{k}n}\hat{a}_{\mathbf{k}n}}_{H_{\mathrm{ph}}} + \underbrace{\sum_{\nu,\sigma,j} E_{\mathbf{k}\nu\sigma j}\hat{b}^\dagger_{\mathbf{k}\nu\sigma j}\hat{b}_{\mathbf{k}\nu\sigma j}}_{H_{\mathrm{ex}}} + \underbrace{i\sum_{n,\nu,\sigma,j} C_{\mathbf{k}n\nu\sigma j}(\hat{a}_{\mathbf{k}n}+\hat{a}^\dagger_{-\mathbf{k}n})(\hat{b}_{-\mathbf{k}\nu\sigma j}-\hat{b}^\dagger_{\mathbf{k}\nu\sigma j})}_{H_I^{(1)}} + \underbrace{\sum_{\mathbf{k},nn',\nu,\sigma,j} D_{\mathbf{k}nn'\nu\sigma j}(\hat{a}_{-\mathbf{k}n}+\hat{a}^\dagger_{\mathbf{k}n})(\hat{a}_{\mathbf{k}n'}+\hat{a}^\dagger_{-\mathbf{k}n'})}_{H_I^{(2)}}.$$

$$C_{\mathbf{k}n\nu\sigma j} \simeq -i\left(\frac{\hbar^2 e^2}{4m_0\varepsilon_0}\frac{f_\sigma}{S}\right)^{\frac{1}{2}}\sum_{\mathbf{G}}\hat{e}_\sigma\cdot\mathbf{E}_{\mathbf{k}+\mathbf{G},n}(z_j)F^*_{\mathbf{k}+\mathbf{G},\nu,\sigma,j},$$

$$D_{\mathbf{k}nn'\nu\sigma j} = C^*_{\mathbf{k}n\nu\sigma j}C_{\mathbf{k}n'\nu\sigma j}/E_{\mathbf{k},\nu,\sigma,j},$$



Parameters: $a = 245$ nm, $d = 64$ nm, $t_u = 184$ nm etched for $t_{etch} = 75.5$ nm, $t_b = 20$ nm, $t_{qw} = 20$ nm, $t_u = 111$ nm. Permittivities: $\varepsilon_{GaAs} = 3.56^2 + 10^{-4}i$, $\varepsilon_{AlGaAs} = 3.32^2$, $\varepsilon_{SiO_2} = 1.45^2$. The quantum well contains a 2D exciton layer with $\frac{f}{S} = 10^{17}$ m^{-2}, $E_{exc} = 1.53$ eV, $\gamma_{exc} = 10$ μeV.



Conclusions

- ✓ The guided-mode expansion is a fast and versatile method for treating photonic crystal slabs and light-matter interaction.
- ✓ It is an approximate method whose range of validity should be carefully checked. It works best for low air fractions and low losses (high Q-factors).
- ✓ `Legume` is free [5], fully python coded, and interfaced with Autograd for inverse design. The final results should best be validated with an exact method (FEM, FDTD, RCWA).
- ✓ The possibility to treat exciton-photon interaction, leading to PhC polaritons, adds a powerful tool for the design of active photonic structures.

References

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