Automated optimization of photonic crystal slab cavities

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Thanks to their high quality factor, combined to the smallest modal volume, defect-cavities in photonic crystal slabs represent a promising, versatile tool for fundamental studies and applications in photonics. In particular, the L3, H0, and H1 defects are the most popular and widespread cavity designs, due to their compactness, simplicity, and small mode volume. For these cavities, the current best optimal designs still result in Q-values of a few times 10⁵ only, namely one order of magnitude below the bound set by fabrication imperfections and material absorption in silicon. Here, we use a genetic algorithm to find a global maximum of the quality factor of these designs, by varying the positions of few neighbouring holes. We consistently find Q-values above one million – one order of magnitude higher than previous designs. Furthermore, we study the effect of disorder on the optimal designs and conclude that a similar improvement is also expected experimentally in state-of-the-art systems.

Photonic crystal (PhC) cavities are a quintessential element of integrated photonic devices. Thanks to ultra-high quality factors and mode volumes close to the diffraction limit, these devices hold promise in a wide range of applications including non-classical light generation, all-optical computational paradigms, solid-state cavity quantum electrodynamics, and sensing. Starting from a two-dimensional PhC consisting of a lattice of air holes etched in a dielectric slab, an optical cavity can be created by introducing a point-like defect – e.g. one or few missing or shifted holes – in the otherwise periodic structure.

A major effort during the last decade has been devoted to the optimization of these structures, in particular through the maximization of the quality factor Q and the minimization of the volume V of the cavity mode, as optical nonlinearities, Purcell effect, and radiation-matter coupling all depend directly on Q and inversely on V². To this purpose, three different approaches can be broadly defined. The first is the inverse problem approach, where an effective equation for the dielectric profile is defined starting from the desired shape of the cavity mode, through a semi-analytical formalism. The second is the topology optimization method, where variations of the entire topology of the PhC are allowed, and the objective function (either Q or Q/V) is maximized numerically. Although some of these works have achieved remarkably high values of Q and Q/V, the resulting cavity designs often pose serious technological challenge in terms of manufacturability, as they present excessively small holes or holes with irregular pattern and sharp features. A third and completely different strategy consists in optimizing simple PhC cavity designs by tweaking only a few geometrical parameters (e.g. by shifting the positions and varying the radii of nearby holes), in order to preserve the small spatial footprint and ease of fabrication of the design. This approach has produced encouraging results, in particular for the three most widespread cavity designs, namely the L3 cavity, the H0 cavity (also known as “zero-cell” or “point-shift” cavity), and the H1 cavity. It brought in some cases an increase of the quality factor by more than one order of magnitude – reaching values of a few hundred-thousands, or even above one million for the H1 hexapole mode – while the mode volume was only slightly increased or sometimes even reduced. A common feature of all these optimization works however is the lack of an exhaustive exploration of the parameter space in search of a global maximum of the objective function.

Experimentally, the quality factor of PhC cavities is limited by extrinsic losses, due to absorption and fabrication imperfections. More precisely, the measured quality factor Qₑ can be expressed as

\[
\frac{1}{Q_e} = \frac{1}{Q_t} + \frac{1}{Q_a} + \frac{1}{Q_d},
\]

where Qₑ is the theoretical quality factor expected from the ideal structure, while 1/Qₐ and 1/Q₅ are measures of the additional loss rates due to material absorption and to disorder-induced extrinsic losses respectively. For silicon PhCs and wavelengths in the 1.5 μm range, record values of Qₑ ranging between one and five million were
measured on cavity designs based on a modulation of a one-dimen- 
sional PhC waveguide\(^{35,38-41}\). For these designs, \(Q_L\) ranges between 2 \(\times\) 10\(^8\) and 10\(^9\), suggesting a value of several millions for both \(Q_L\) and \(Q_r\). While displaying a mode volume up to three times larger than that of defect cavities, these waveguide-based designs have a consid-
erably larger footprint. There are no fundamental reasons that 
should prevent the quality factor of the most popular defect cavities 
from reaching values of several million, close to the current bound set 
by disorder and absorption.

Here, we adopt a simple optimization strategy. Similarly to several 
existing works\(^{23,24,48,11,13,15,33,34}\), we choose a small set of variational 
parameters – typically the spatial shifts of a few holes next to the defect – 
thus producing designs that can be easily realized with current nano-
fabrication processes. Differently from these works however, we 
carry out a global exploration of the parameter space by means of an 
evolutionary algorithm. Here, by “global” we mean the exhaustive 
search for the global maximum of the quality factor in the parameter 
space of choice. In this way we demonstrate that it is possible to 
 systematically optimize L3, H0, and H1 cavities to values of \(Q_L\) well 
above 10\(^8\) – typically more than one order of magnitude above pre-
vious optimal values – without a large increase of the mode volumes.

The key to this drastic improvement is the exhaustive search, that 
finds configurations overlooked by previous approaches, as exem-
plified by the simplest of the two L3 designs considered here. This 
optimization procedure is made computationally feasible thanks to 
the use of the guided-mode expansion (GME) method\(^{39}\), that allows 
calculating the modes and quality factors of each variation within 
minutes of computational time. Thanks to this computational advantage, we also statistically analyze the influence of fabrication 
imperfections on the optimal designs and conclude that a consid-
erable improvement in the experimental quality factor can be 
expected, as recently demonstrated for the H0 design\(^{34}\).

**Results**

The cavities studied here are formed in a triangular lattice with pitch 
\(a\) of air-holes of radius \(R\) etched in a silicon (\(n = 3.46\)) slab of 
thickness \(d\). In what follows, all lengths will be expressed in units 
of \(a\), as the quality factor is invariant upon a spatial rescaling of the 
structure. We however set parameters such that, for the typically used 
thickness \(d = 220\) nm, the resonant modes lie in the telecommuni-
cation band around \(\lambda = 1.55\) \(\mu\)m. For the simulation of a single 
structure, we use the GME method\(^{40}\) (see Methods). This method 
has already proven reliable for modelling high-Q cavities\(^{35,37}\). As 
a further check of its validity, the results for all final (optimized) struc-
tures are verified using the 3-D finite-difference time-domain 
(FDTD) method\(^{40}\) (see Methods). For each of the optimized designs 
presented here, we also analyse the probability density of \(Q_L\), in the 
presence of fabrication imperfections (and neglecting the absorption 
loss contribution 1/\(Q_L\)). The disorder model is that of Gaussian 
distributed random fluctuations in the position and radius of each hole, 
with zero mean and standard deviation \(\sigma\) (which is a measure of the 
disorder magnitude). Disorder in all holes in the computational cell 
was included, and no hole-hole correlations were taken into account. 
Irregular hole shapes can in general easily be included, but the result-
ing effect is well described by an effective radius fluctuation\(^{41}\). The 
disorder model thus captures well what is accepted as the main 
source of losses in silicon photonic crystal cavities\(^{34,35,38,36}\).

The first cavity design we investigate is the widely-employed L3 
cavity formed by three missing holes in a row (Fig. 1(a)), with \(d = 0.55a\) 

and \(R = 0.25a\). The quality factor of this cavity has already been 
optimized\(^{38,42}\) with respect to shifts of the positions of three neighbour-
hing holes (marked \(S_{1x}, S_{2x}, S_{3x}\) in the Figure), by using a simpli-
fied approach in which, starting from the unshifted design, each of the 
three shifts has been varied once while keeping the two others 
constant. To explore the extent to which this approach is suitable, we 
compute a full map of the quality factor on a relevant region of the 
\((S_{1x}, S_{2x}, S_{3x})\)-space. The map is displayed in Fig. 1(b)–(m). There, 
in each panel, \(Q_L\) is plotted as a function of \(S_{2x}\) and \(S_{3x}\), while the value of 
\(S_{1x}\) increases from 0.15a to 0.37a in steps of 0.02a when going from 
panel (b) to panel (m). Technically, these plots already provide a 
global optimization of the cavity (a clear maximum of \(Q_L\) can be 
identified), although performed in the least practical, brute-force 
way. If applied to the panels of Fig. 1 (though approximately, given 
the coarse \(S_{1x}\) step used in this figure), the simplified optimization 
procedure in Ref. 2 leads to the point marked by a white cross in panel 
(e) (more precisely, \(S_{1x} = 0.21a, S_{2x} = 0.01a, S_{3x} = 0.23a\)), i.e. far off 
the maximum that can be seen in panel (k) at \(S_{1x} = 0.33a, S_{2x} = 0.26a, S_{3x} = 0.10a\). It is also interesting to note that within the range of the plots in Fig. 1(b–m), two maxima are visible - a local one 
around \(S_{1x} = 0.25a, S_{2x} = 0.09a, S_{3x} = 0.21a\) in panel (g) and another 
which first appears at \(S_{1x} = 0.29a, S_{2x} = 0.18a, S_{3x} = -0.10a\) in panel 
(i) and then shifts to become the global maximum at \(S_{1x} = 0.327a, S_{2x} = 0.257a, S_{3x} = 0.116a\). In general, even an even larger 
number of local extrema might in principle be present, especially for larger 
number of parameters, thus making the search for the global 
extrimum more difficult. This highlights the need for a global optim-
ization procedure instead of a more conventional algorithm (e.g. the 
conjugate gradient) that would almost inevitably find a local rather 
than a global maximum.

Ideally, we would like to apply a global, stochastic (since there is no 
general way to come up with a “good” guess for a starting point) 
procedure to the problem of optimizing the cavity parameters. Thus, 
we choose to employ a genetic algorithm which typically relies on a 
range of evolution-inspired techniques to create consecutive “gen-
erations” of cavities each containing better and better “individuals”, 
until convergence is reached. This type of algorithm proves very 
efficient especially with increasing number of free parameters. We use 
the genetic algorithm provided in the MATLAB\(^{\text{\textregistered}}\) Global 
Optimization Toolbox (see Methods), where we choose the objective 
function to be the GME-computed quality factor \(Q_L\). When applied to 
the L3 with freedom in \(S_{1x}, S_{2x}, S_{3x}\), the optimal design is found for 
\(S_{1x} = 0.337a, S_{2x} = 0.257a\) and \(S_{3x} = 0.116a\) (Fig. 2(a)). This 
yields \(Q_L = 2.1 \times 10^9\) (FDTD: 1.6 \(\times\) 10\(^9\)), which is an increase by a factor of \(\approx 6\) as compared to the previously highest value\(^2\) of 3.3 \(\times\) 10\(^9\) (FDTD: 2.6 \(\times\) 10\(^9\)), while the mode volume (see Methods) 
increases from 0.77(\(\mu\)m\(^3\)) to 0.94(\(\mu\)m\(^3\)). One obvious advantage of 
using evolutionary optimization rather than the brute-force para-
meter scan of Fig. 1 is the precision with which the maximum can 
be pinpointed; another one is that a few tens of generations with a 
population of 80 individuals are sufficient to reach this converged 
configuration (see Methods). Moreover, the design can be further 
improved if two more shifts (\(S_{4x}\) and \(S_{5x}\) in Fig. 1(a)) are allowed in 
the optimization, which is still easily handled by the genetic algo-
ithm, although \(\approx 100\) generations are needed for convergence. 
In this case, the optimized design is found for \(S_{1x} = 0.337a, S_{2x} = 0.270a, S_{3x} = 0.088a, S_{4x} = 0.233a,\) and \(S_{5x} = 0.173a\) (Fig. 2(b)), and 
has \(Q_L = 5.1 \times 10^9\) (FDTD: 4.2 \(\times\) 10\(^9\)) with mode volume \(V = 0.95(\mu\text{m})^3\), i.e. an increase in \(Q_L\) by one order of magnitude compared to the previous optimal values\(^3,8\), with an increase in the mode 
volume comparable to the three-shift case. The resonant frequency 
of the modes is at \(\omega a / 2\pi c = 0.259\) for both designs, which is slightly 
lower than the frequency \(\omega a / 2\pi c = 0.263\) of the unmodified L3 (i.e. with 
the same \(d/a\) and \(R/a\) but with no hole shifts).

The choice of just these few free parameters is not unique, but 
appears optimal. Attempts were made at including other position 
shifts or radii variations of the holes surrounding the cavity defect, 
which however did not bring to a significant further increase in \(Q_L\). 
Having only a few hole shifts as free parameters results in a tech-
nologically friendly structure, and in a more compact cavity defect, 
characterized by a much smaller footprint on the PhC, than wave-
guide-based ultrahigh-Q designs\(^4,8,9\). In addition, the present designs
are as robust to fabrication imperfections as any other high-$Q$ PhC cavity, as can be inferred from Fig. 2(c)–(f). In panel (c) we plot, for the three-shift L3, the dependence of $Q_t$ on $S_{2x}$ and $S_{3x}$ as in Fig. 1, but for the value $S_{1x} = 0.327a$ corresponding to our optimal design (the white cross indicates where the design lies with respect to $S_{2x}$ and $S_{3x}$). In this plot, we observe that the width of the maximum is larger than the typical uncertainty in the hole positions (smaller than $0.005a$ for Si 42). Furthermore, in Fig. 2(d)–(e) we show, respectively for the three- and five-shift design, the computed probability of occurrence of $Q_t$-values in presence of disorder. Each of these histograms was obtained by simulating 1000 disordered realisations of the corresponding cavity design. The blue plot in panel (d) in particular shows that for a state-of-the-art disorder magnitude $\sigma = 0.0015a$ (i.e. about $0.6$ nm 12,25, when assuming $a = 400$ nm in a silicon slab), the average value lies at about $Q_t = 2.5 \times 10^6$, i.e. quality factors one order of magnitude larger than the previous theoretical maximum can be expected in practice, highlighting the significance of the design optimization. Finally we note that, for a given set of optimal values of the $S_{nx}$ parameters, the designs are also robust to small changes in the overall hole radius $R$ and slab thickness $d$, that can originate from an offset in the fabrication process and/or be introduced on purpose in order to e.g. tune the resonant frequency to a desired value. To show this, in panel (f) we plot the value of $Q_t$ obtained by varying $R$ and $d$ while keeping the shifts $S_{1x} = S_{3x}$ constant and set to the values obtained for the optimal design computed at $d = 0.55a$ and $R = 0.25a$. We observe that $Q_t > 4 \times 10^6$ for a range of $R$ and $d$ values which is much larger than the fabrication uncertainty and which allows fine-tuning of the frequency. For certain values of $d$ and $R$ (to the right of the dashed line in the Figure), higher-order guided modes of the slab become non-negligible. More precisely, a TM-like band of the regular PhC becomes resonant with the cavity mode and introduces a new loss channel 38. We point out that, while $Q_t$ appears to systematically increase with $d$ in the single-mode region, it drops rapidly as soon as $d$ increases into the multi-mode region. An ana-

Figure 1 | (a): The design of the L3 cavity. For quality factor optimization, shifts of the positions of the five neighbouring holes in the $x$-direction were introduced, labeled as $S_{1x}$, $S_{2x}$, $S_{3x}$, $S_{4x}$ and $S_{5x}$ in the figure. (b)–(m): A parameter scan of the GME-computed quality factor values for different $S_{1x}$, $S_{2x}$ and $S_{3x}$, where $S_{1x}$ starts from $0.15a$ in panel (b) and increases in multiples of $0.02a$ in every consecutive panel, up to $0.37a$ in (m), and $S_{4x} = S_{5x} = 0$ in all panels.
logous trend of the loss rates as a function of $R/a$ and $d/a$ is expected for the other cavity designs discussed in this study. In principle, one could consider $d/a$ and/or $R/a$ as free parameters in the optimization, but in that case setting a target wavelength, for a fixed value of $d$ that might arise from technological requirements, becomes more difficult.

Often, obtaining the highest possible theoretical $Q_c$ is not the main goal of optimization. In fact, when $Q_c$ gets above a limit set by the material and the fabrication process (currently $\approx 5 \times 10^6$ in silicon\cite{si}), the experimentally measured $Q_c$ is always dominated by losses due to disorder and/or absorption, and so weakly affected by further increase in $Q_c$. The potential of an automated optimization procedure is therefore best exploited when applied to other attractive properties. One example consists in maximizing $Q_t$ while having the smallest possible mode volume, so that $Q/V$ is as high as possible, since the latter is a figure of merit for applications in both cavity QED\cite{cqed,si} and non-linear optics\cite{nl}. With this in mind, the second design we focus on is the H0 cavity\cite{zero} (sometimes also named “zero-cell” or “point-shift”), namely the simple defect cavity with the smallest known mode volume.

The design of the H0 is shown in 3(a); the defining defect is the shift of two holes away from each other (S1x), the thickness of the slab taken here is $d = 0.5a$, while the hole radius is $R = 0.25a$. For the optimization, we also use the consecutive shifts $S_{2x} - S_{3x}$, as well as two shifts in the vertical direction, $S_{1y}$ and $S_{2y}$. Using $S_{1x}, S_{2x}, S_{3x}, S_{1y}$ and $S_{2y}$, the cavity has already been optimized\cite{optim} (following the same approach already discussed for the L3) to a quality factor of $Q_t = 2.8 \times 10^6$, with a corresponding mode volume $V = 0.23(\lambda/n)^3$. Here, we improve on this result by on one hand using the genetic optimization, and on the other by including $S_{3x}$ and $S_{5x}$. It should be mentioned that in the optimization, an allowed range of variation for each parameter is set. For the H0, we find that the maximum allowed $S_{1x}$ is a very important parameter, increasing which produces several different optimized designs. All of those are interesting, as increasing $S_{1x}$ increases the mode volume but also the $Q_c$ of the cavity. More precisely, the designs in 3(b)–(d) were obtained by imposing the following restrictions in the genetic algorithm: $S_{1x} = 0.25a$, $S_{1z} \leq 0.3a$, and $S_{1x} \leq 0.4a$, respectively. The ensuing optimal parameters $[S_{1x}, S_{2x}, S_{3x}, S_{1y}, S_{2y}, S_{3y}, S_{4y}, S_{5y}]$ are as follows: $[0.216a, 0.103a, 0.123a, 0.040a, 0.194a, -0.017a, 0.067a]$ (panel (b)); $[0.280a, 0.193a, 0.194a, 0.162a, 0.113a, -0.016a, 0.134a]$ (panel (c)); and $[0.385a, 0.342a, 0.301a, 0.229a, 0.116a, -0.033a, 0.093a]$ (panel (d)). The corresponding quality factors are $Q_t = 1.04 \times 10^6$ (FDTD: $1.04 \times 10^6$), $Q_t = 1.88 \times 10^6$ (FDTD: $1.66 \times 10^6$), and, remarkably, $Q_t = 8.89 \times 10^6$ (FDTD: $8.29 \times 10^6$), while the respective mode volumes are $V = 0.25(\lambda/n)^3$, $V = 0.34(\lambda/n)^3$, and $V = 0.64(\lambda/n)^3$. The first among these three designs (panel (b)) has a mode volume only slightly larger than the previous most optimal design, combined to a quality factor almost four times larger. The last of the three designs (panel (d)) instead shows a more significant increase of the mode volume, but associated with respect to the value obtained in Ref. 6. The resonance frequencies of the three designs decrease with the increase of $V$ and are $\omega_a / 2\pi c = 0.280$, $\omega_a / 2\pi c = 0.275$, and $\omega_a / 2\pi c = 0.269$, respectively, while the original cavity with $S_{1x} = 0.14$ (and no other shifts) of Ref. 9 has $\omega_a / 2\pi c = 0.292$.

Similarly to what we have done above for the L3 cavity, in Fig. 3(e)–(g) we present the probability of occurrence of $Q_c$ values, computed using 1000 random disorder realizations for each design and each disorder magnitude. From these histograms it appears clearly that, even though design 3 has the highest theoretical $Q_c/V$, it might not be the best choice in practice. According to Eq. (1) in fact, depending on the amount of disorder, the maximum value of the
actual ratio \(Q_e/V\) will in general be achieved for a design having an intermediate value of \(Q_e\). For example, in the case with \(\sigma = 0.003 a\) (red curves in panels (e)–(g)), the average values of \(Q_e\), neglecting absorption computed from the simulations are \(3.97 \times 10^5\), \(5.23 \times 10^5\), and \(6.49 \times 10^5\), respectively, meaning that the highest \(Q_e/V\) would in practice be achieved by design 1. On the other hand, for the smaller disorder \(\sigma = 0.0015 a\) (blue curves in panels (e)–(g)), the corresponding average values of \(Q_e\) are \(7.22 \times 10^5\), \(1.12 \times 10^6\), and \(2.02 \times 10^6\), and the highest average \(Q_e/V\) is achieved by design 2. For both values of \(\sigma\), the expected \(Q_e/V\) for the five-shift L3 cavity is lower than that for any of the three H0 designs, thus the latter should be the cavity of choice for applications where a quantum dot is placed in the center of the cavity. Here, we optimize the quality factor of the dipole mode. We take \(d = 0.55 a\) and \(R = 0.23 a\), and the parameters used for design optimization, labeled \(S_1\), \(S_2\), and \(S_3\) in Fig. 4(a), are an increase in the side-length of the three consecutive hexagonal “rings” around the cavity (which is also equivalent to the increase of the distance from a vertex of a hexagon to the cavity center). The previously most-optimal design was achieved using only the holes at the vertices of the hexagons (but including variations of the hole radii), and has a moderate \(Q_e = 6.2 \times 10^5\) and a mode volume \(V = 0.47 (\lambda/n)^3\). Here, using the genetic algorithm with the shifts as outlined in Fig. 4(a), we find an optimal design at \(S_1 = 0.213 a\), \(S_2 = 0.070 a\), and \(S_3 = 0.009 a\), with \(Q_e = 1.05 \times 10^6\) (FDTD: \(0.97 \times 10^6\)) and \(V = 0.62 (\lambda/n)^3\), i.e. we find a 19-fold increase in \(Q_e\) coupled to an increase in \(V\) by 32%. For this cavity as well, the disorder analysis (panel (d)) suggests that \(Q_e\) values close to a million can be expected experimentally in state-of-the-art silicon systems, i.e. more than an order of magnitude larger than the previous theoretical values. The modes lie at a frequency \(\omega a/2\pi c = 0.253\), which is, as expected, slightly lower than that of the unmodified cavity, \(\omega a/2\pi c = 0.270\).

We note that while the degeneracy of the two dipole modes is an attractive feature of the H1, it is lifted by disorder. This is why, in panel (e) of Fig. 4, we study the probability of occurrence of the splitting between the modes, based on the 1000 disorder realizations that were used for the disorder analysis in panel (d). It is important to note that there is no absolute way to define an \(x-y\) reference frame, as three equivalent frames (rotated 60° from one another) exist due to the hexagonal symmetry of the cavity. This symmetry is broken if the cavity presents preferential orientations of the axes (e.g. introduced by lithography). In the case where only random disorder is considered, \(x\)- and \(y\)-polarized modes can turn out to be oriented along either of the three \(x-y\) reference frames. Thus, what we plot in panel
The designs obtained here for the three most widespread PhC defect-cavities consistently show that the quality factor of these cavities can be systematically optimized to well above $10^6$ by adjusting only a few structural parameters (only shifts of hole positions were used here), with small increases in the mode volumes (within 50% with the exception of the third H0 design) as compared to those of the corresponding non-optimized designs. In carrying out our analysis, we have tried to include the radii of holes next to the cavity as additional free parameters, but this brought no significant improvement. We therefore restricted to shifts of hole positions only, as these are easily controlled in the fabrication process. Our scheme leaves the possibility open to use the hole radii as free parameters for independent optimization of some additional figure of merit.

A very important conclusion of our analysis is that the parameter space of such structural variations has to be explored globally, using an automated optimization tool. We find that the genetic algorithm is an excellent tool to handle this task, even when seven parameters are included in the computation, as was the case for the H0 cavities.

Employing this algorithm was possible only due to the computational advantage of the GME – to compute the number of cavity configurations that was needed for the optimization using a first-principle tool like FDTD or a Finite-Element Method (FEM) would require either an enormous computational power, or time of the order of years. This computational advantage made it also possible, for each cavity type, to vary more structural parameters than in previous optimization works, thus bringing to an even larger increase in the quality factors. Finally, we note that the GME returns not only the GME returns not only the statistical analysis of $Q$-factors but also the full mode profile of the cavity modes, thus the same procedure which was presented here can be used for optimization of different quantities depending on the practical requirements, like $Q/V$ for applications in non-linear optics, or optimal electric field profiles for e.g. sensing technologies, which we expect to explore in the next future.

The statistical analysis of $Q$-factors including structural disorder shows clearly that the designs obtained here are as robust to disorder as other ultrahigh-$Q$ designs. In particular, for the L3 cavity with a theoretical $Q$-factor $Q_t = 5.1 \times 10^6$, state-of-the-art fabrication quality in silicon should easily result in experimental $Q$-factors around $2 \times 10^6$, in the same range as current ultrahigh-$Q$ designs based on a PhC waveguide. On the other hand, our experience shows that systematic structural variations can rapidly suppress the $Q$-factor of
an optimal structure. Hence, an important conclusion of our analysis is that, whenever a design needs to be significantly varied (e.g. when strongly modifying the ratios R/a or d/a, or the refractive index n in order to, e.g., operate at a different wavelength), a new optimization must be carried out in order to obtain the best structural design adapted to the new requirements.

The range of applicability of the present scheme is very broad. We are currently applying it to several systems, including the optimization of the Q-factor of PhC cavities with low index contrast\(^{39}\), of cavities based on a thicker slab (d/a > 1, typically needed to host some quantum nanostructures\(^{39}\)), but also to the maximization of the trapping capabilities of slot cavities designed for biological sensing\(^{36}\), and to the simultaneous optimization of first and second order modes of a cavity built in a PhC structure with doubly resonant bandgap for efficient second-harmonic generation\(^{51}\). In all these cases, the global optimization brought to very promising results. A further application might include the optimization of PhC structures based on a silicon-on-insulator design\(^{22,43}\). Perhaps even more importantly, our work has general implications about the future research in photonic crystals, as it shows that the domain of possible structural designs is still largely unexplored, while simultaneously demonstrating how its exploration can be done efficiently.

Methods

The guided-mode expansion. The GME method used in this work\(^{36}\) is based on expanding the mode of a cavity on the basis of the guided modes of an effective dielectric slab. In the z-direction (orthogonal to the slab plane), the whole space from minus to plus infinity is included analytically; in the slab plane, a finite super-cell is taken and periodic boundary conditions are assumed. The super-cell size in our simulations ranges from \(L_x = 16a\) to \(L_x = 20a\) in the x-direction and from \(L_y = 12(\sqrt{3}a/2)\) to \(L_y = 20(\sqrt{3}a/2)\) in the y-direction, depending on the cavity. The supercell naturally defines a grid of in-plane wave-vectors \(G = 2\pi(n_l/L_x, n_m/L_y)\) (with integer \(n_l\) and \(n_m\)) each of them labeling a wave guided inside the slab and evanescent along the z-direction. The expansion is carried out onto a truncated set of \(N_G\) such waves (centered at \(G = 0\)) and the number \(N_G\) is increased until convergence is reached (typically \(N_G \geq 5000\)). For all the optimizations, only the fundamental (\(z = 1\) in Ref. 38) guided mode is used, since for the thickness assumed here, the admixture to the maximum is reached for the H0 cavity with 7 parameters, for which \(300 \times 300\) generations each consisting of 129 individuals are needed for convergence. This can however be greatly improved if a rough optimization is first carried out (with a large allowed range for the free parameters), followed by a finer optimization centered around the rough maximum. The longest optimization we ran thus took about a week on twelve CPUs with 32 GB of RAM. This would have taken more than ten years to finish using the same machine but employing an FDTD solver instead of the GME.

Mode volume. Here we adopt the definition of the mode volume that is most commonly used to quantify the performance of a nanocavity:

\[
V = \int \frac{|r(r)|^2 |E(r)|^2}{\max[|r(r)|^2 |E(r)|^2]} \, dr
\]

This definition is the one needed in cavity quantum electrodynamics as a measure of the radiation-matter coupling with a pointlike two-level system placed at the position where the field intensity has a maximum. Other definitions are more suited to different purposes and might in some cases differ dramatically from the one above\(^{21}\).

FDTD simulations. For the FDTD simulations, we use the freely available MIT Electromagnetic Equation Propagation (MEEP) package\(^{40}\). Typical simulations parameters are supercell size 40a in the x-direction and 30(\(\sqrt{3}a/2\)) in the y-direction, and spatial resolution 20/\(a\). Taking advantage of the parallelized (MPI) version of the software, a converged computation takes of the order of ten hours on a 16-core processor with 32 GB of RAM. A more detailed comparison of computational time and accuracy between GME, FDTE and the Finite-Element Method (FEM) can be found in Ref. 37.

Genetic optimization. The implementation of the genetic algorithm included in the Global Optimization Toolbox (MATLAB and Global Optimization Toolbox Release 12b, The MathWorks, Inc., Natick, Massachusetts, United States), which starts from a random initial population (i.e. a set of points in parameter space) and goes on to create a sequence of generations (new sets of such points) where the ‘fittest’ individuals are kept. The algorithm incorporates an array of evolutionary inspired techniques, including cross-over, random mutations, and natural selection of individuals. An ‘individual’ in our case is simply one Q-computation for a particular set of cavity parameters, and the higher the quality factor, the higher the assigned ‘fitness’ of the individual (i.e. its probability to survive to the next generation and/or to be mixed with another individual to produce an ‘offspring’ lying in parameter space somewhere in between the two). With the increase of the number of free parameters, the number of generations needed for convergence increases. In the presented work, the maximum is reached for the H0 cavity with 7 parameters, for which \(300 \times 300\) generations each consisting of 129 individuals are needed for convergence. This can however be greatly improved if a rough optimization is first carried out (with a large allowed range for the free parameters), followed by a finer optimization centered around the rough maximum. The longest optimization we ran thus took about a week on twelve CPUs with 32 GB of RAM. This would have taken more than ten years to finish using the same machine but employing an FDTD solver instead of the GME.
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Additional information
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