

**Rose K. Cersonsky^{1,a}, James Antonaglia^{2,b},
Bradley Dice^{2,c}, Sharon C. Glotzer^{1,2,3,4,5}**

¹Macromolecular Science and Engineering, University of Michigan

²Department of Physics, University of Michigan

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⁵Biointerfaces Institute, University of Michigan

Current Affiliations:

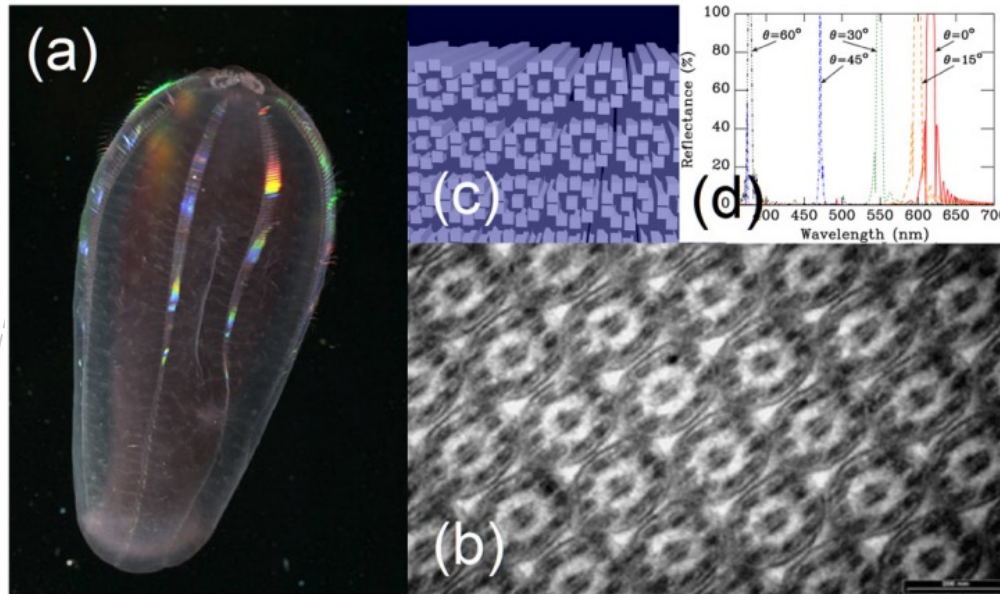
^aLaboratory of Computational Science and Modeling (COSMO),
École Polytechnique Fédérale de Lausanne (EPFL)

^bDivision of Mathematics and Science, Bard Early High School and
College

^cRAPIDS Team, NVIDIA

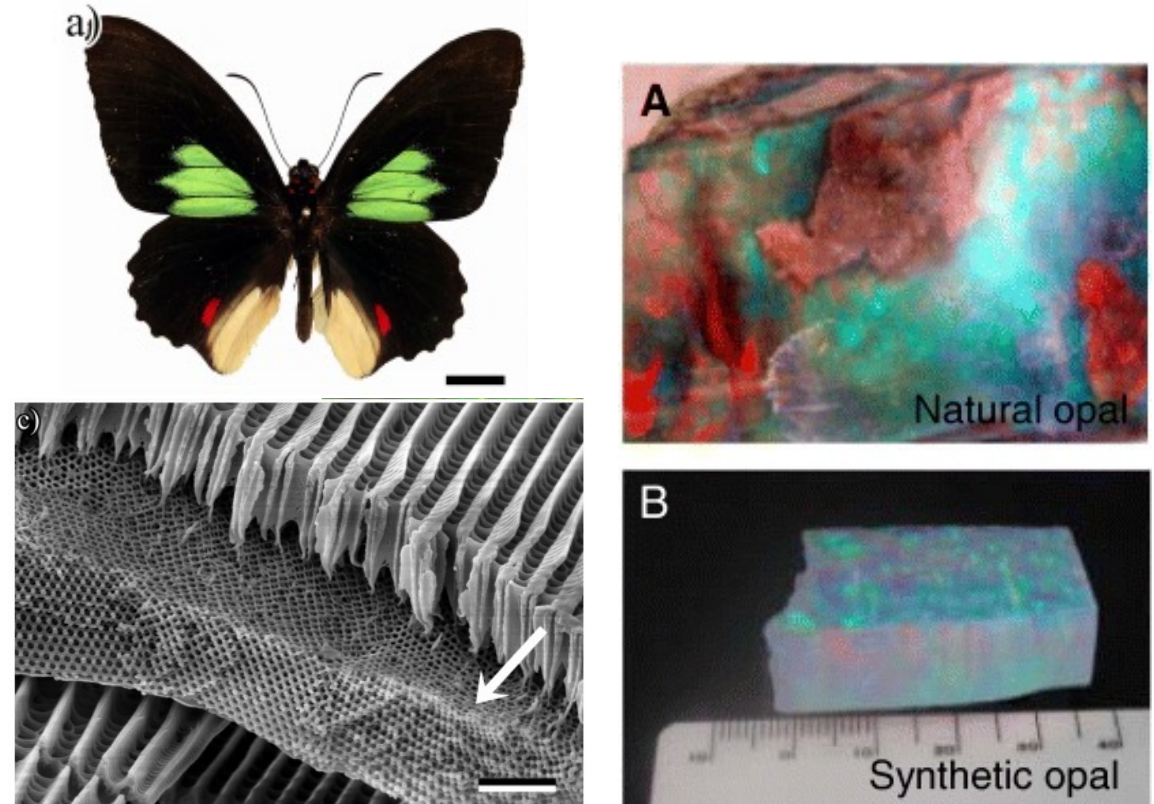
The Diversity of Three- Dimensional Photonic Crystals for Colloidal Self-assembly

Colloidal photonic crystals are responsible for some of the most vibrant and beautiful structural color in nature.



Optical properties of the iridescent organ of the comb-jellyfish *Beroë cucumis* (Ctenophora)

Victoria Welch, *et al.*
Phys. Rev. E 73, 041916 2006



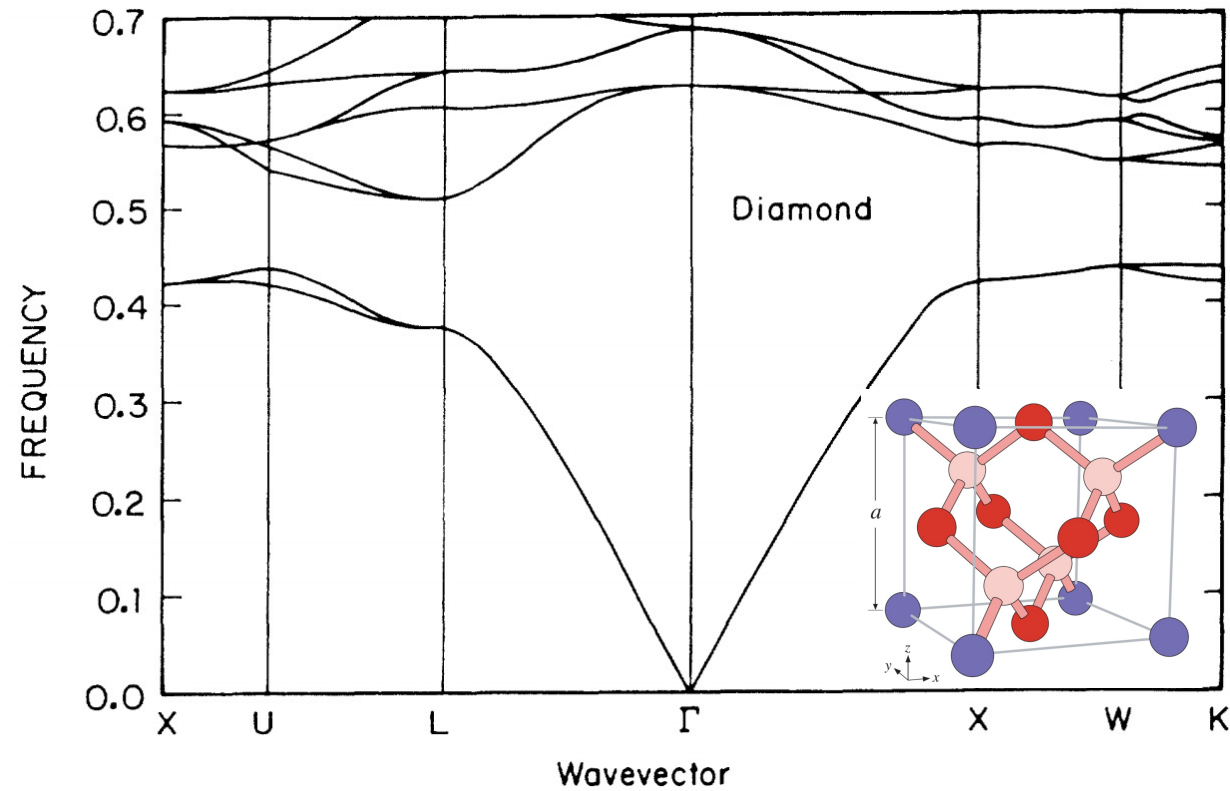
Optical properties of gyroid structured materials: from photonic crystals to metamaterials

James A. Dolan, *et al.*
Advanced Optical Materials 3 (1), 12-32

Tunable structural color in organisms and photonic materials for design of bioinspired materials

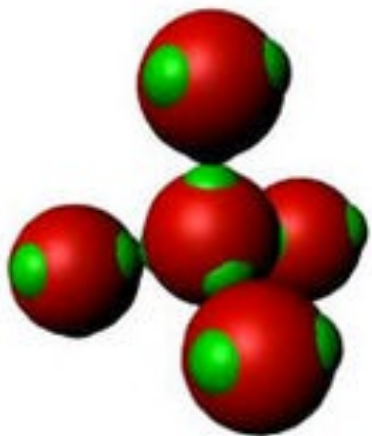
Hiroshi Fudouzi
Sci. Technol. Adv. Mater. (2011) 12 064704

A complete photonic band gap occurs when there are frequencies not transmittable through a mixed-dielectric medium.

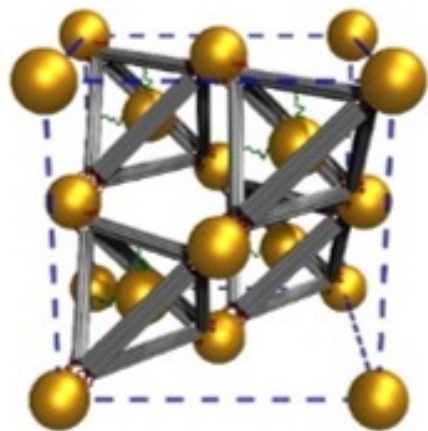


Existence of a Photonic Gap in Periodic Dielectric Structures
K. M. Ho, C. T. Chan, and C. M. Soukoulis
Physics Review Letters 65, 25 (1990)

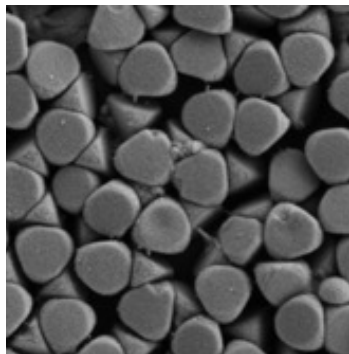
There have been many different approaches to obtain diamond at the colloidal length scale.



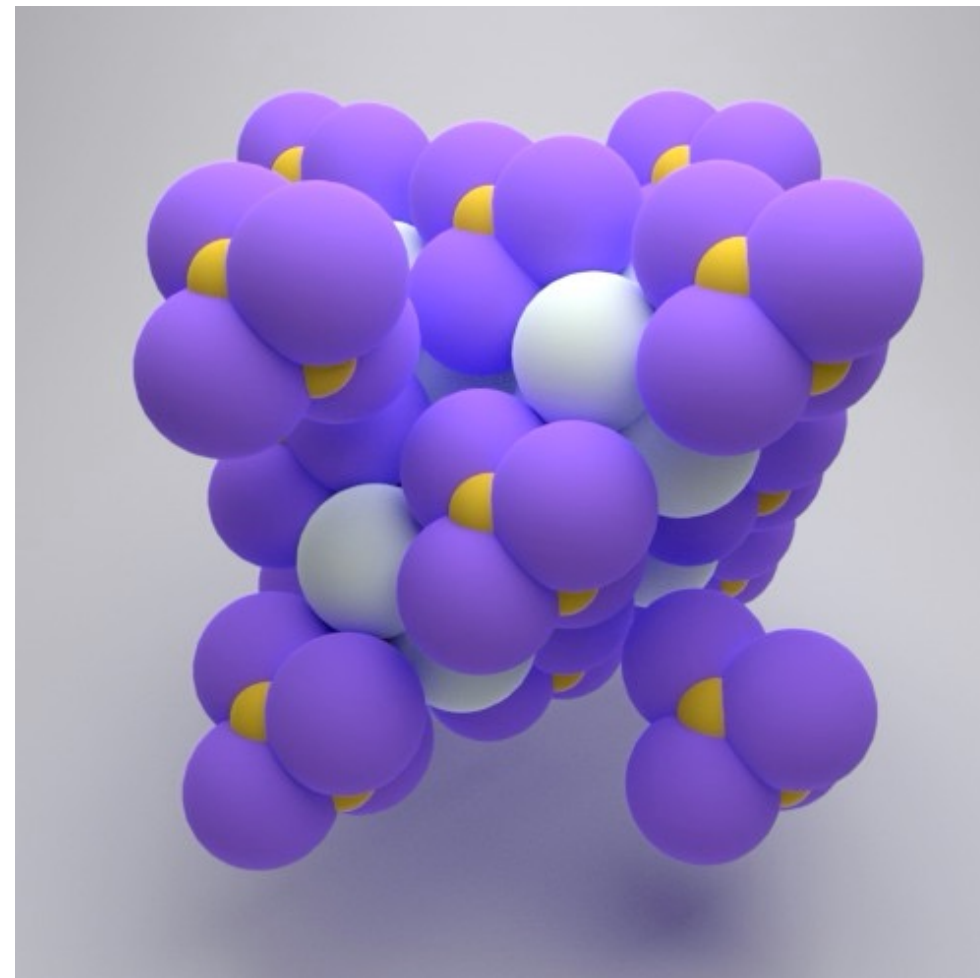
Colloidal crystals with diamond symmetry at optical lengthscales
Yifan Wang, et al.
Nature Comm. 8, 14173 (2017)



Diamond family of nanoparticle superlattices
W. Liu, et al.
Science 351, 582-586 (2016).



Entropy driven assembly of truncated colloidal tetrahedra into diamond structure
Zhe Gong, et al.

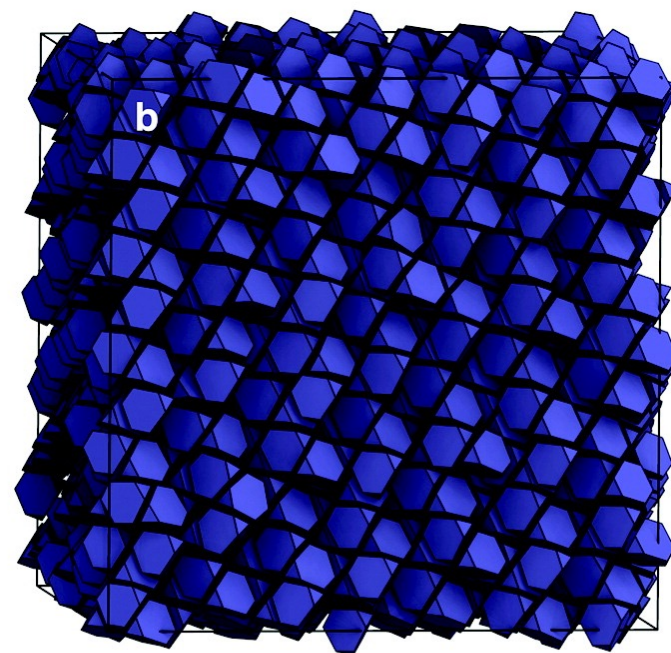


Colloidal Diamond
He, M., et al.
Nature 585, 524-529 (2020).

However, perfect diamond is not necessary to support a complete photonic band gap.

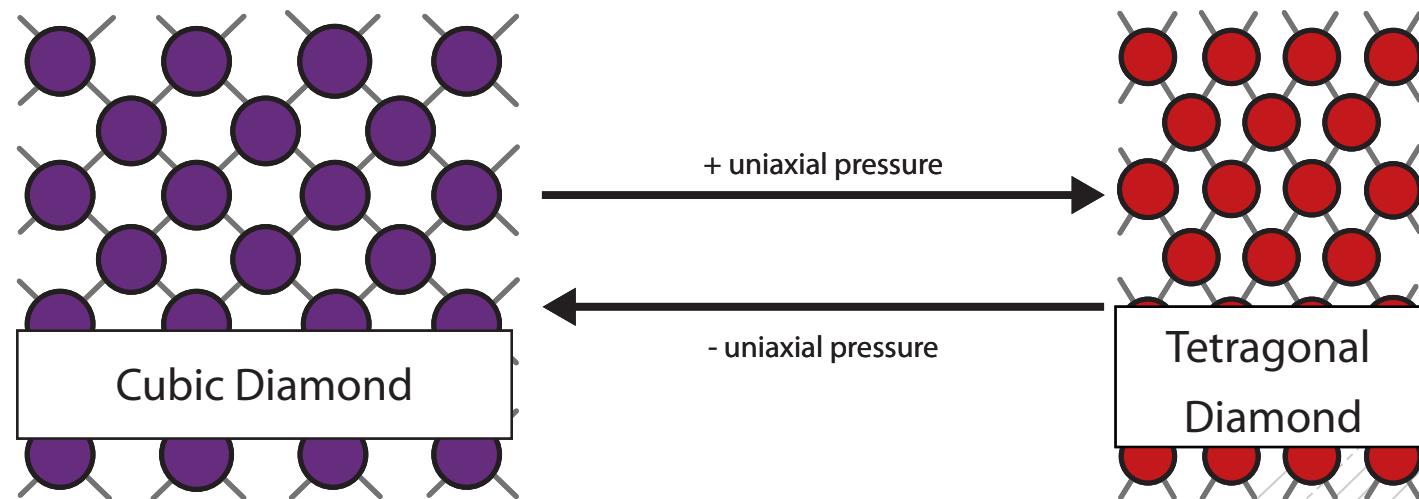
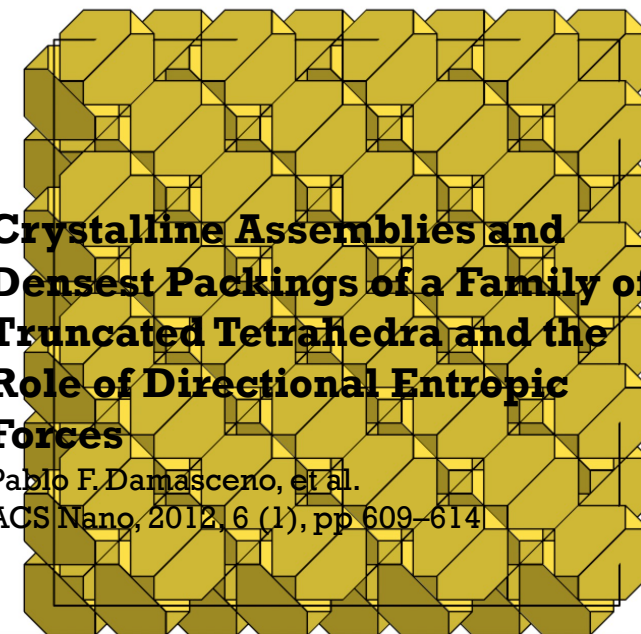
Pressure-tunable photonic band gaps in an entropic colloidal crystal

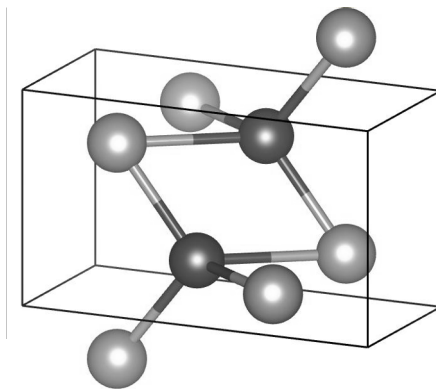
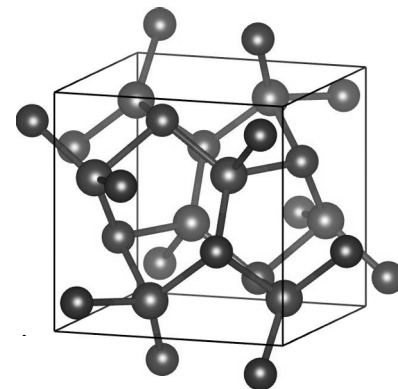
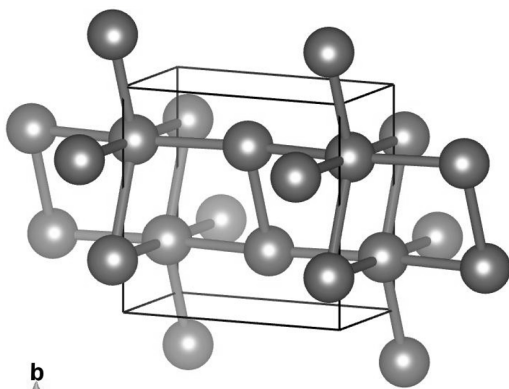
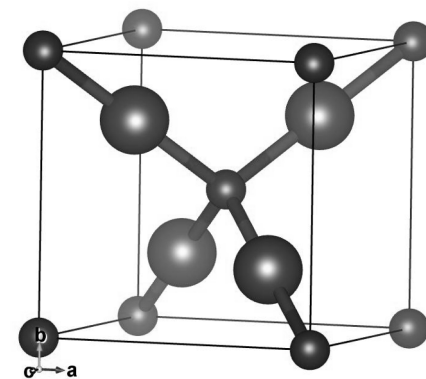
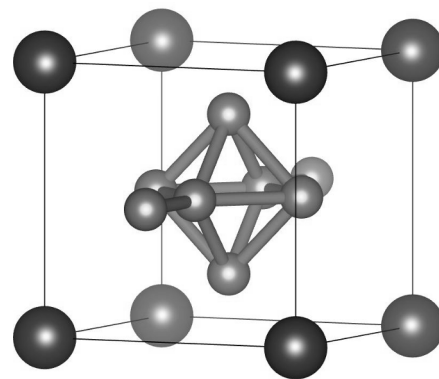
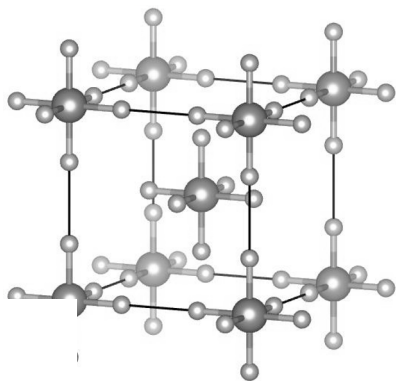
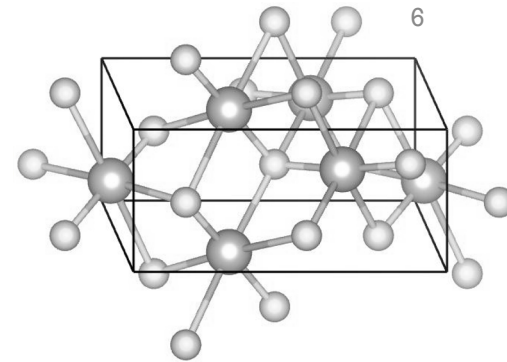
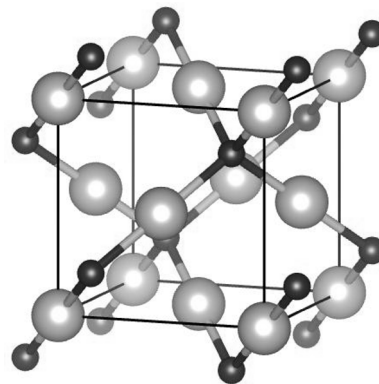
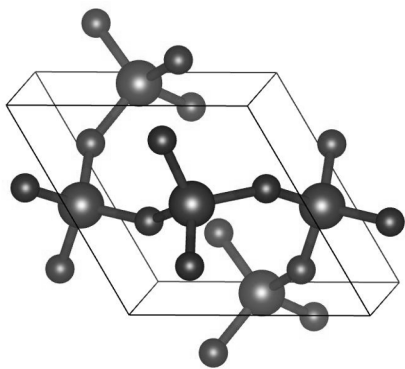
Rose K. Cersonsky Julia Dshemuchadse,
James Antonaglia, Greg van Anders, and Sharon C. Glotzer
Physical Review Materials (2018) 2(12), 125201.
<https://doi.org/10.1103/PhysRevMaterials.2.125201>



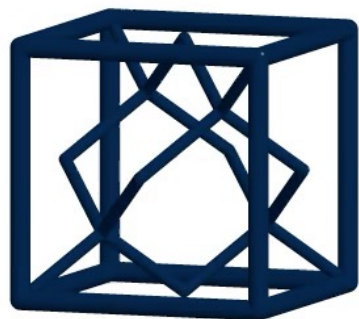
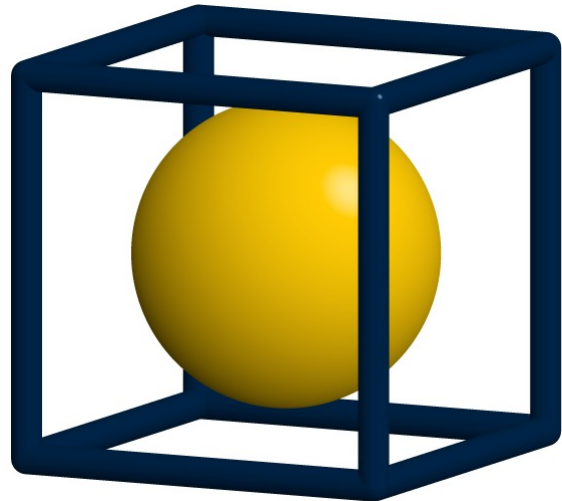
Crystalline Assemblies and Densest Packings of a Family of Truncated Tetrahedra and the Role of Directional Entropic Forces

Pablo F. Damasceno, et al.
ACS Nano, 2012, 6 (1), pp 609–614

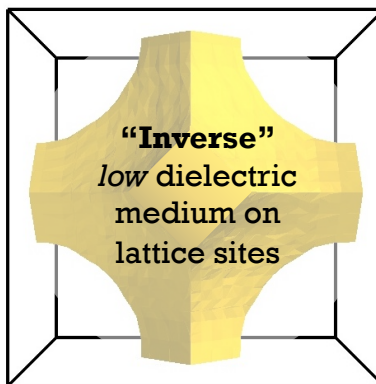
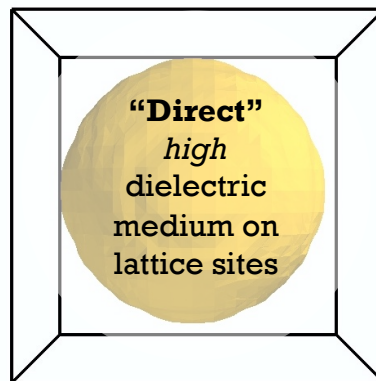




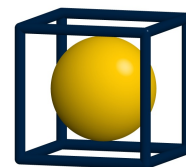
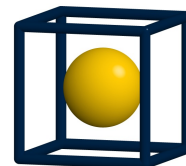
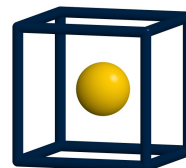
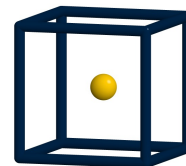
1355 Structure Templates



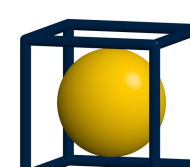
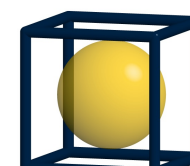
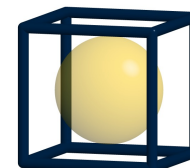
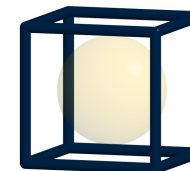
x 2 Instantiations



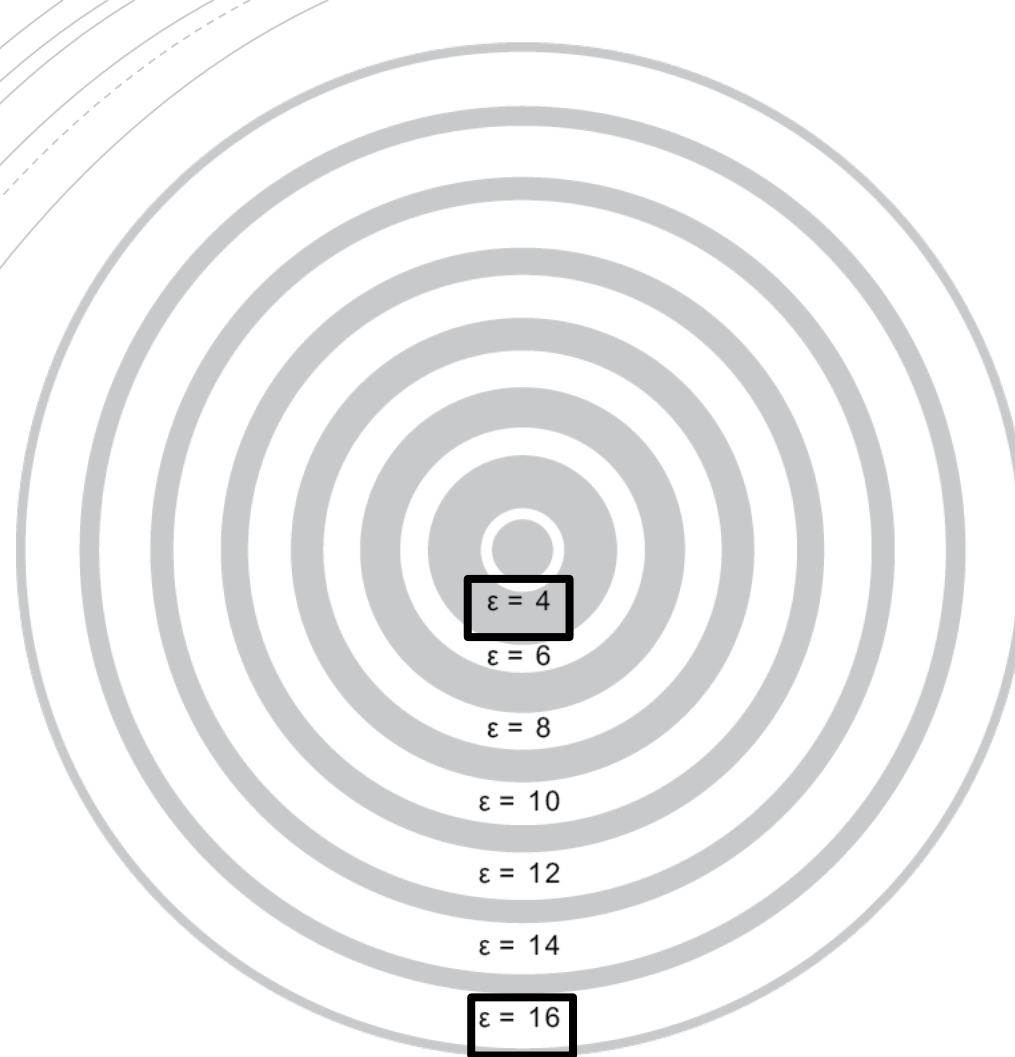
x 20-100 radii



x 1-8 dielectric constants



> 150,000 band structures



Existence of a photonic gap
in periodic dielectric
structures.

Ho, K. M., Chan, C. T. &
Soukoulis, C. M. *Phys. Rev.
Lett.* 65, 3152–3155 (1990).

Robust topology
optimization of three-
dimensional photonic-
crystal band-gap structures.

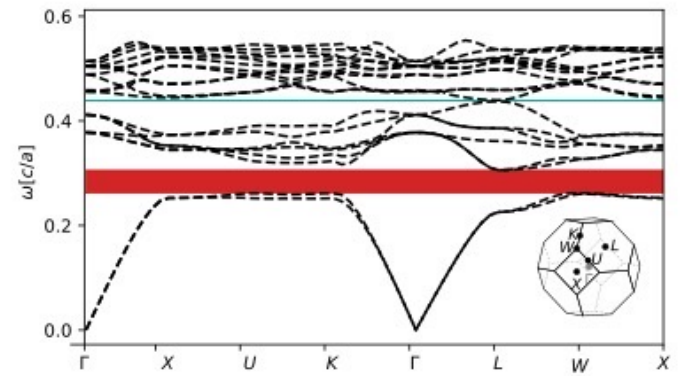
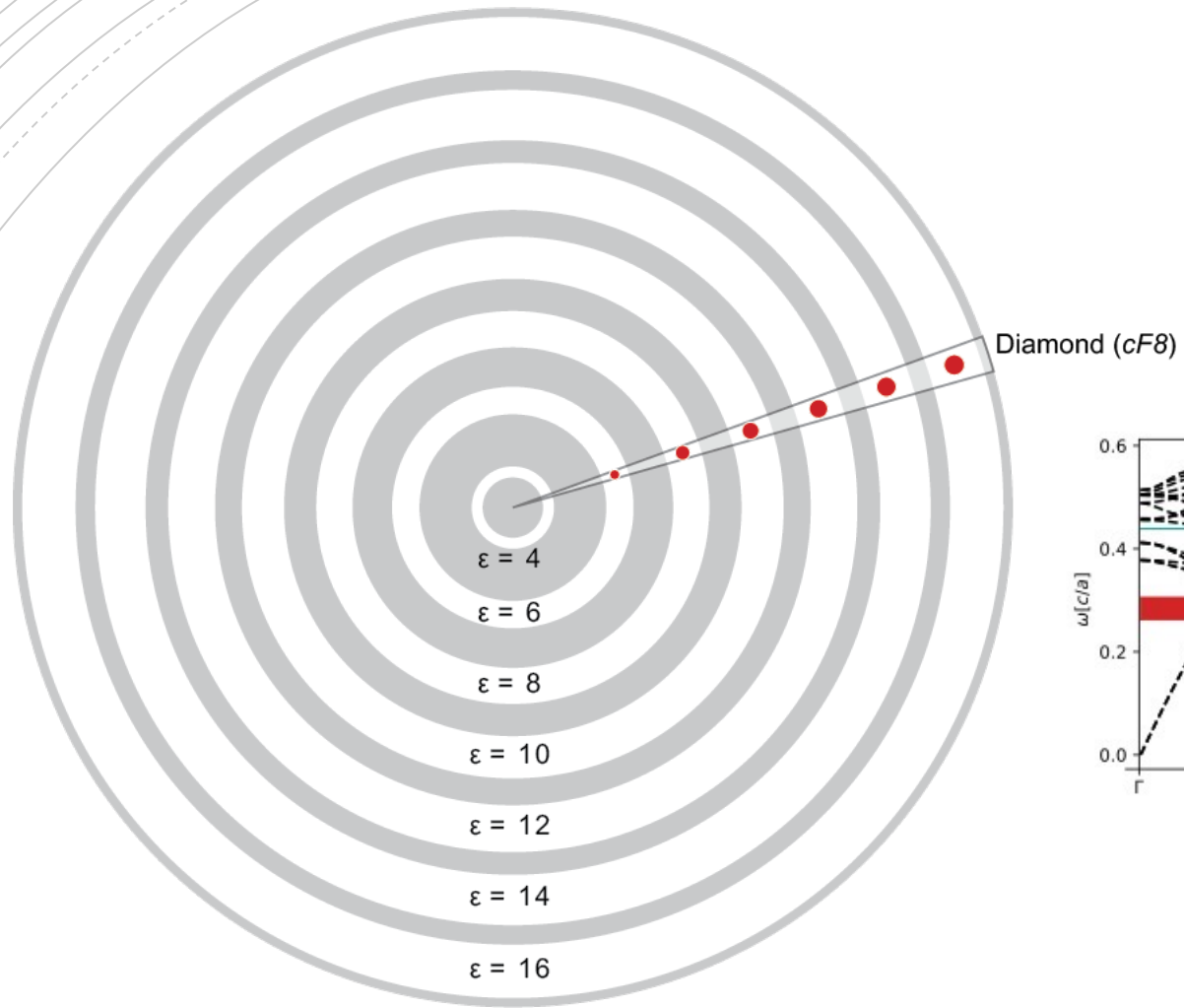
Men, H., Lee, K. Y. K., Freund,
R. M., Peraire, J. & Johnson, S.
G.

Opt. Express 22, 22632
(2014).

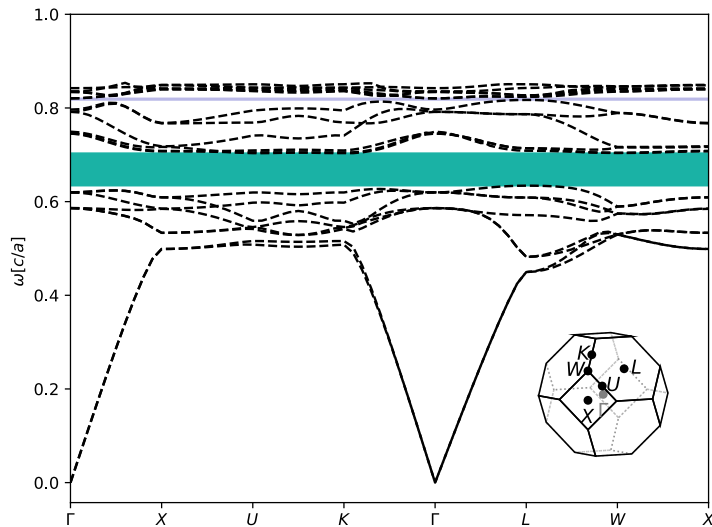
Refractive index of silicon
and germanium and its
wavelength and
temperature derivatives.

Li, H. H. J. *Phys. Chem. Ref.
Data* 9, 561 658 (1980).

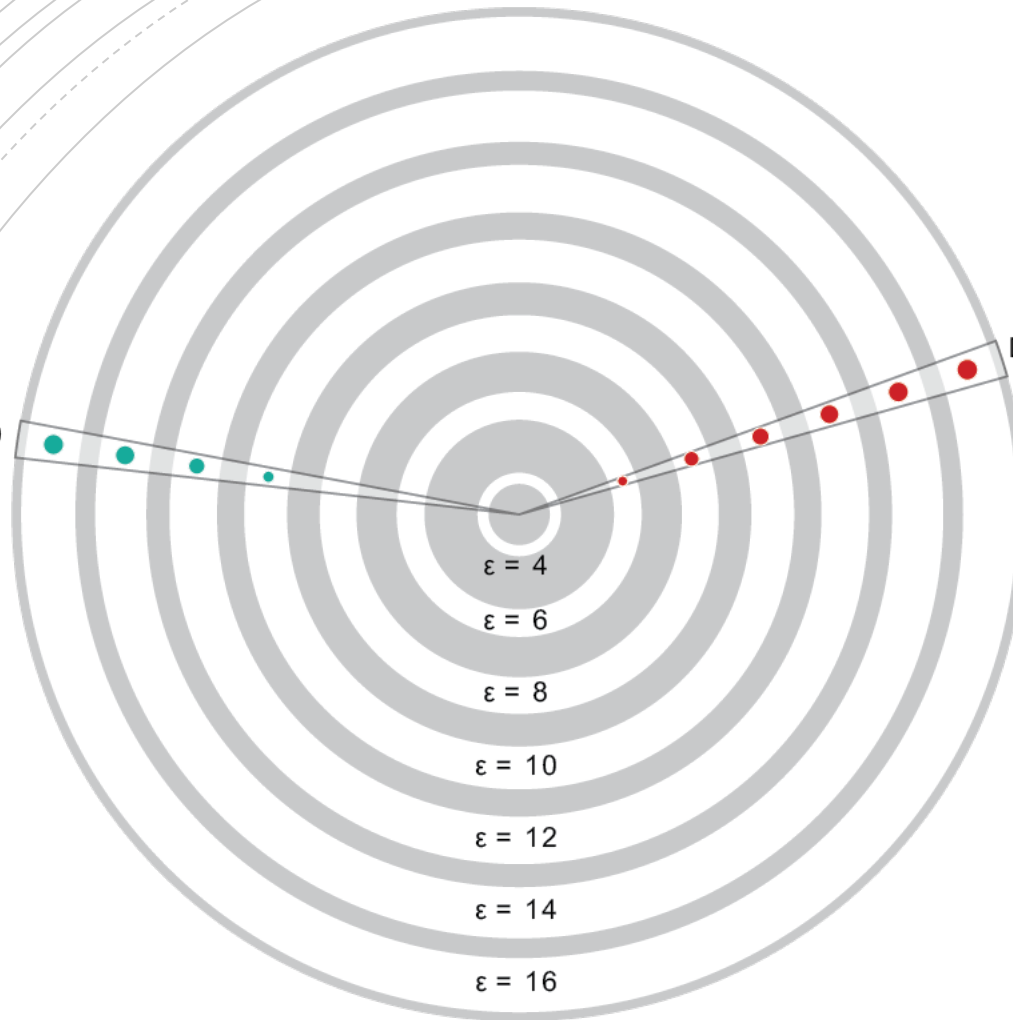
The diversity of three-dimensional photonic crystals
RKC, et al. *Nature Communications* 12,
<https://doi.org/10.1038/s41467-021-22809-6> (2021).



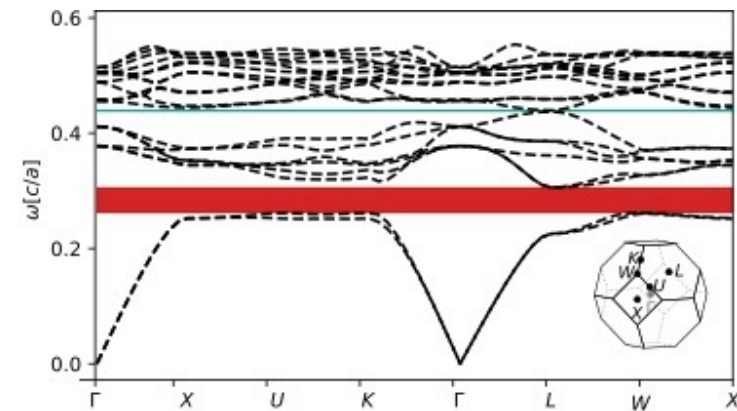
The diversity of three-dimensional photonic crystals
RKC, et al. Nature Communications 12,
<https://doi.org/10.1038/s41467-021-22809-6> (2021).



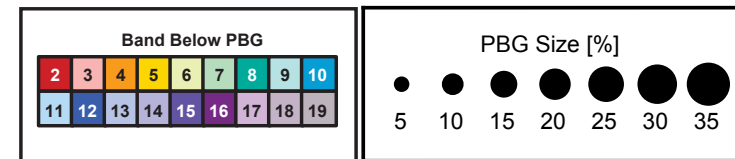
Diamond (cF8)



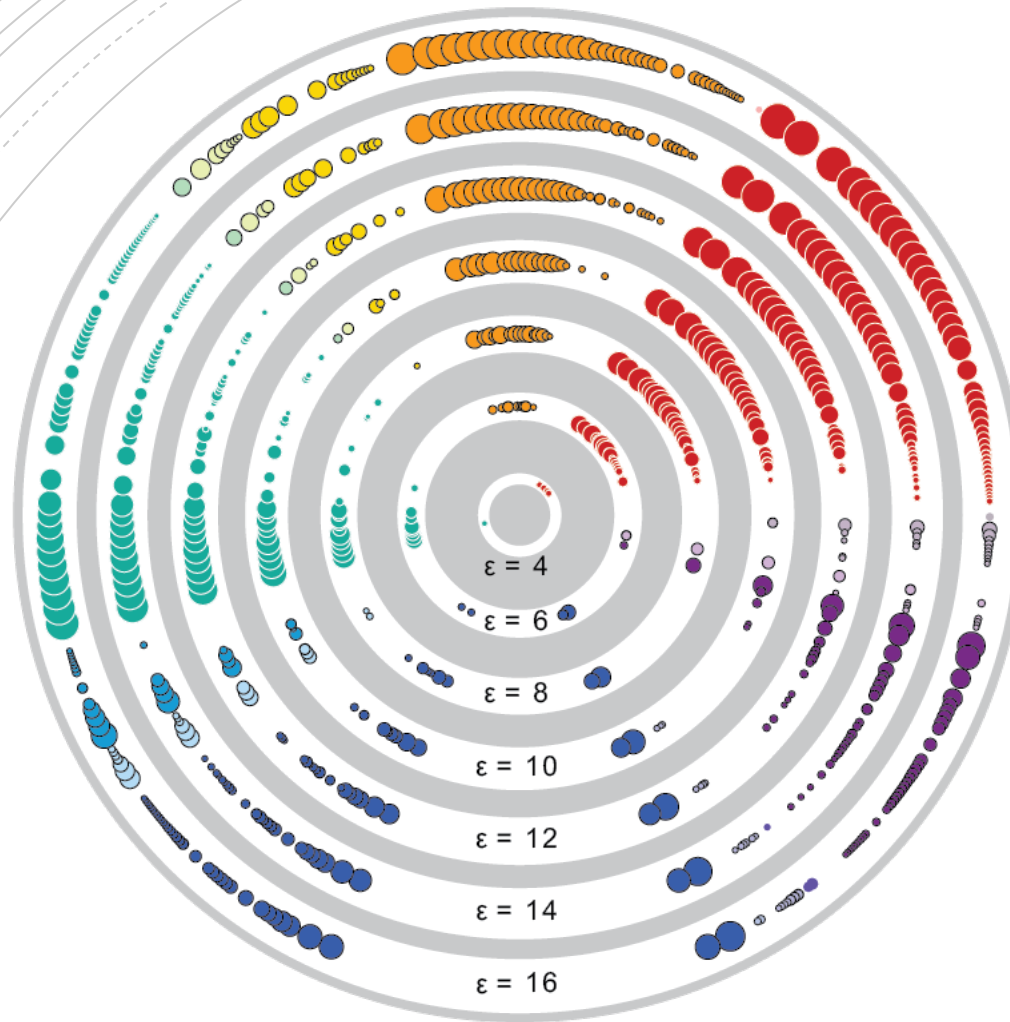
Diamond (cF8)



The diversity of three-dimensional photonic crystals
RKC, et al. Nature Communications 12,
<https://doi.org/10.1038/s41467-021-22809-6> (2021).



Each circle represents the maximum gap (circle size) found for a given template (radius), dielectric contrast (ring), and band location (color).



351 Photonic
“Templates”
(almost 300 *new*
templates)

474 Unique Gaps

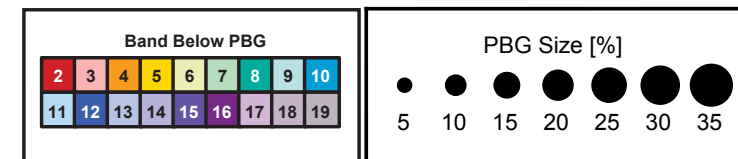
Database of Photonic Crystals:

<https://glotzerlab.engin.umich.edu/potonics/index.html>

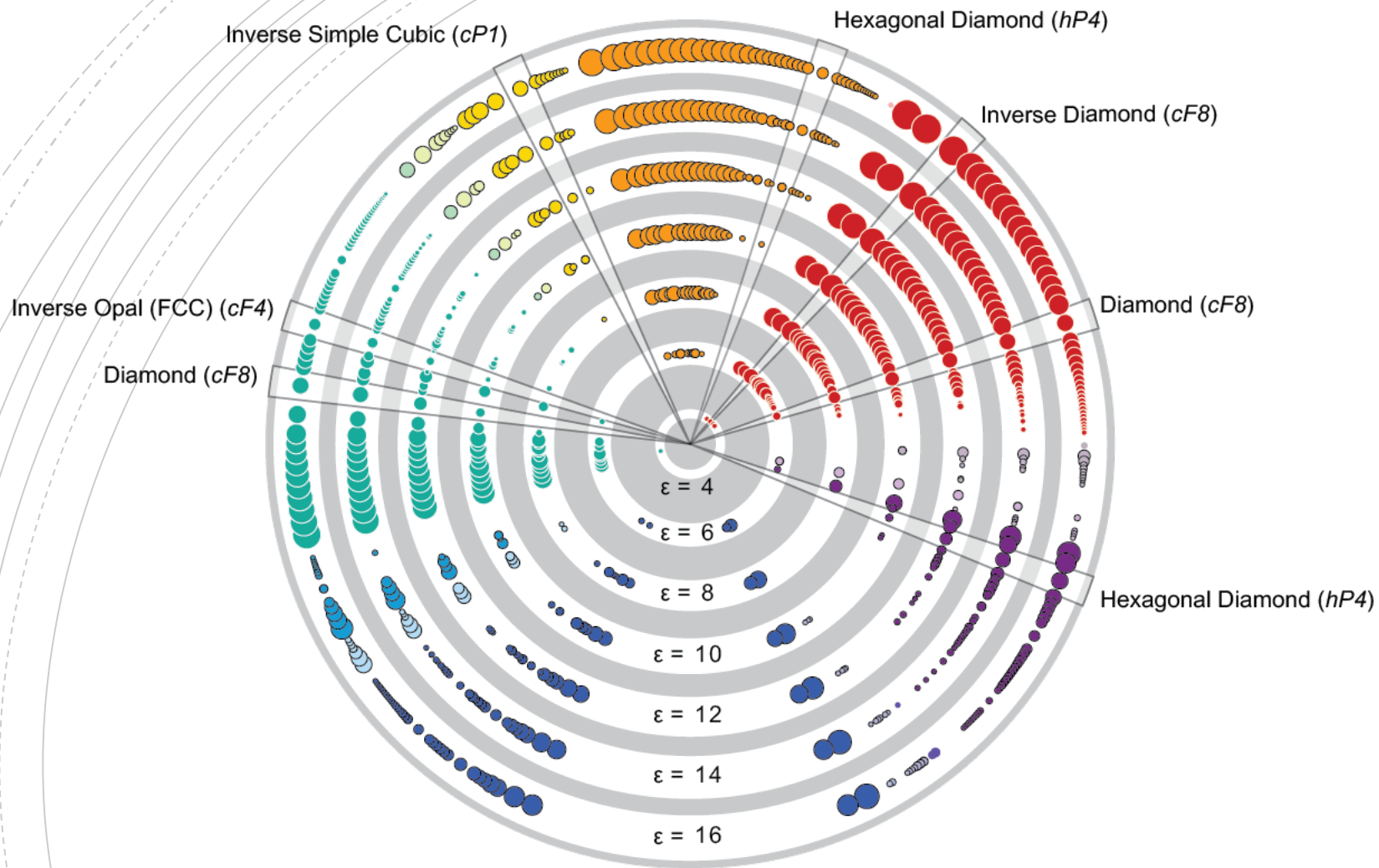
Appendix of Band Structures:

<https://deepblue.lib.umich.edu/handle/2027.42/153520>

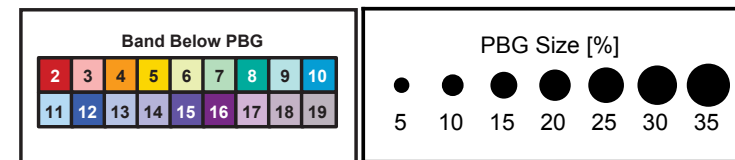
The diversity of three-dimensional photonic crystals
RKC, *et al. Nature Communications* 12,
<https://doi.org/10.1038/s41467-021-22809-6> (2021).



Each circle represents the maximum gap (circle size) found for a given template (radius), dielectric contrast (ring), and band location (color).



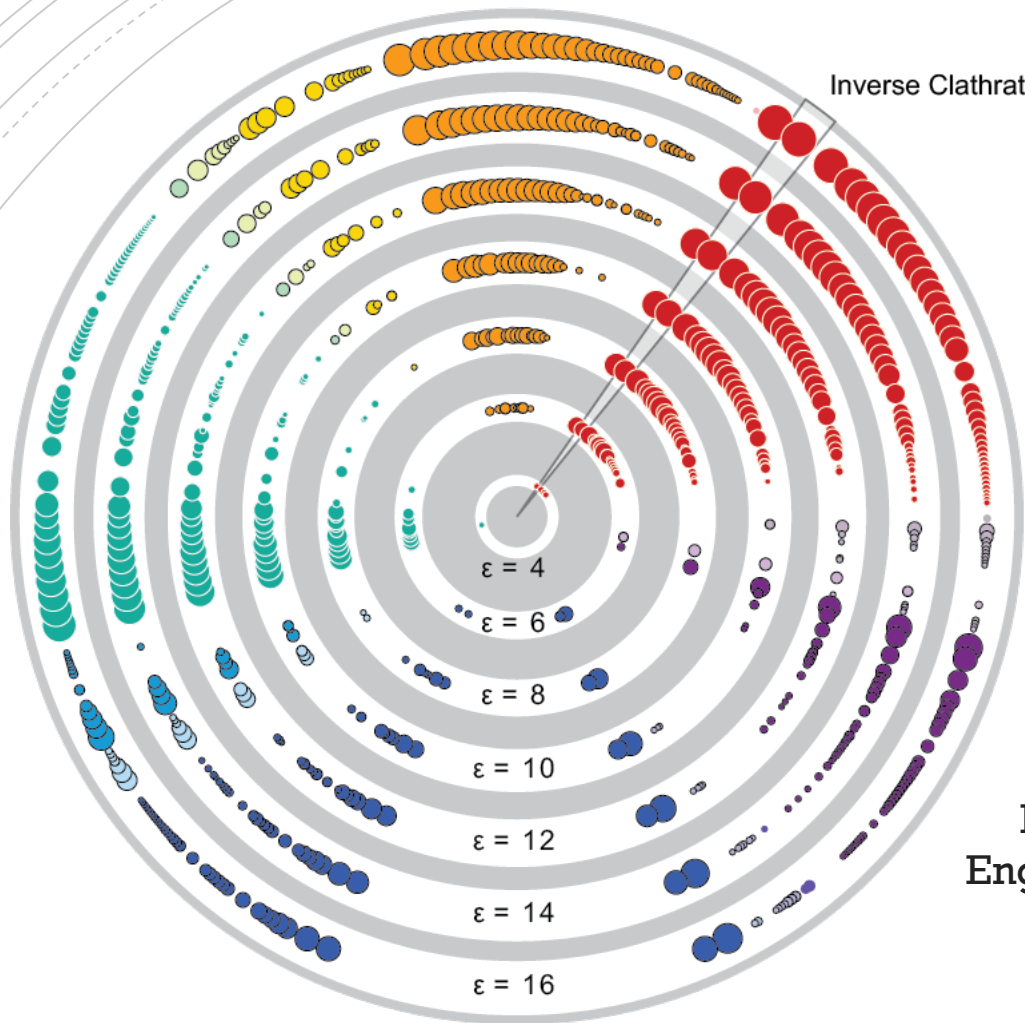
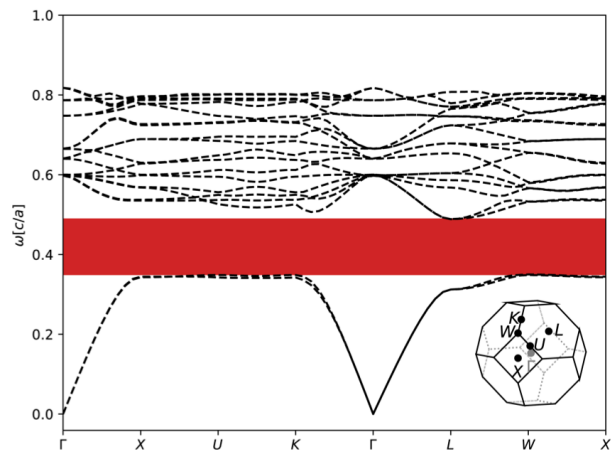
The diversity of three-dimensional photonic crystals
RKC, et al. *Nature Communications* 12,
<https://doi.org/10.1038/s41467-021-22809-6> (2021).



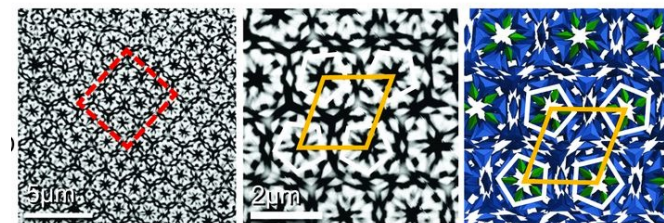
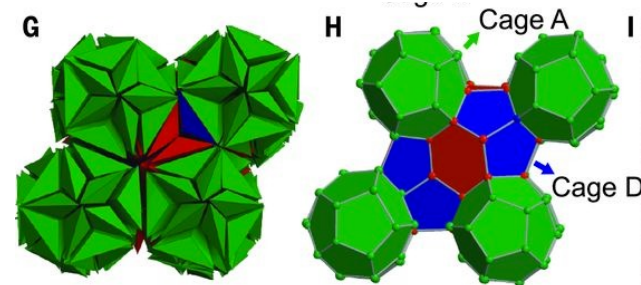
Each circle represents the maximum gap (circle size) found for a given template (radius), dielectric contrast (ring), and band location (color).

Inverse Clathrate-II

Maximum Gap: 33.9%

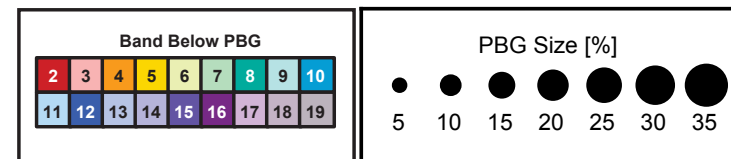


Inverse Clathrate-II (cF136)

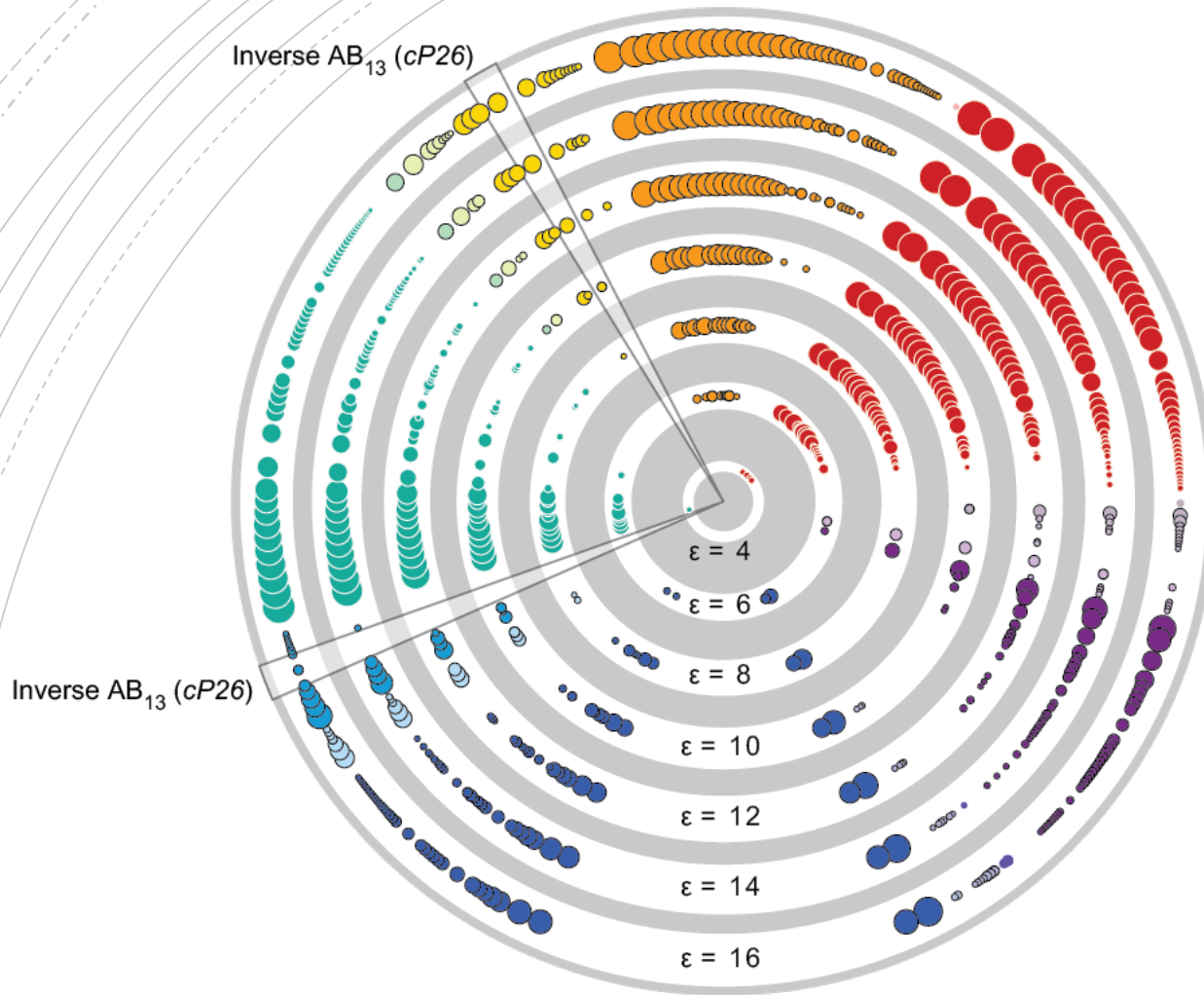


Clathrate colloidal crystals.
 Lin, H., Lee, S., Sun, L., Spellings, M.,
 Engel, M., Glotzer, S. C., & Mirkin, C. A.
 Science, 355(6328), 931-935.

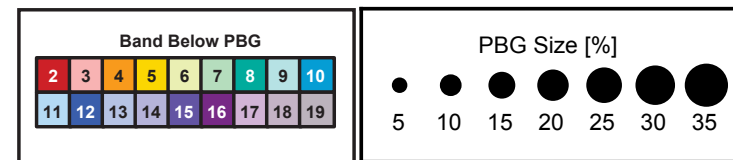
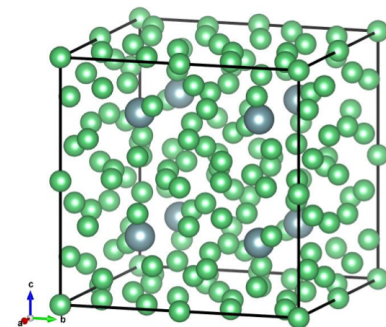
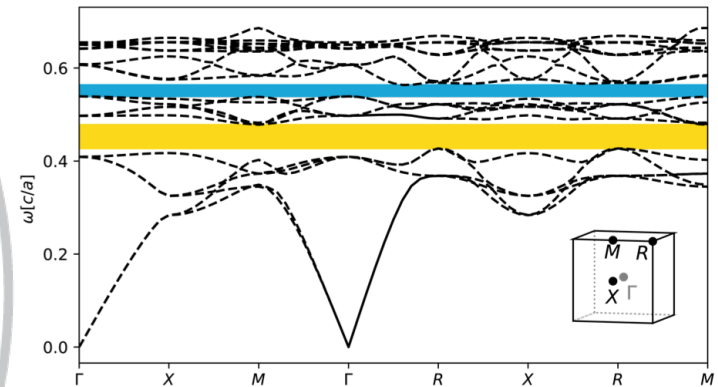
The diversity of three-dimensional photonic crystals
 RKC, et al. *Nature Communications* 12,
<https://doi.org/10.1038/s41467-021-22809-6> (2021).



Each circle represents the maximum gap (circle size) found for a given template (radius), dielectric contrast (ring), and band location (color).

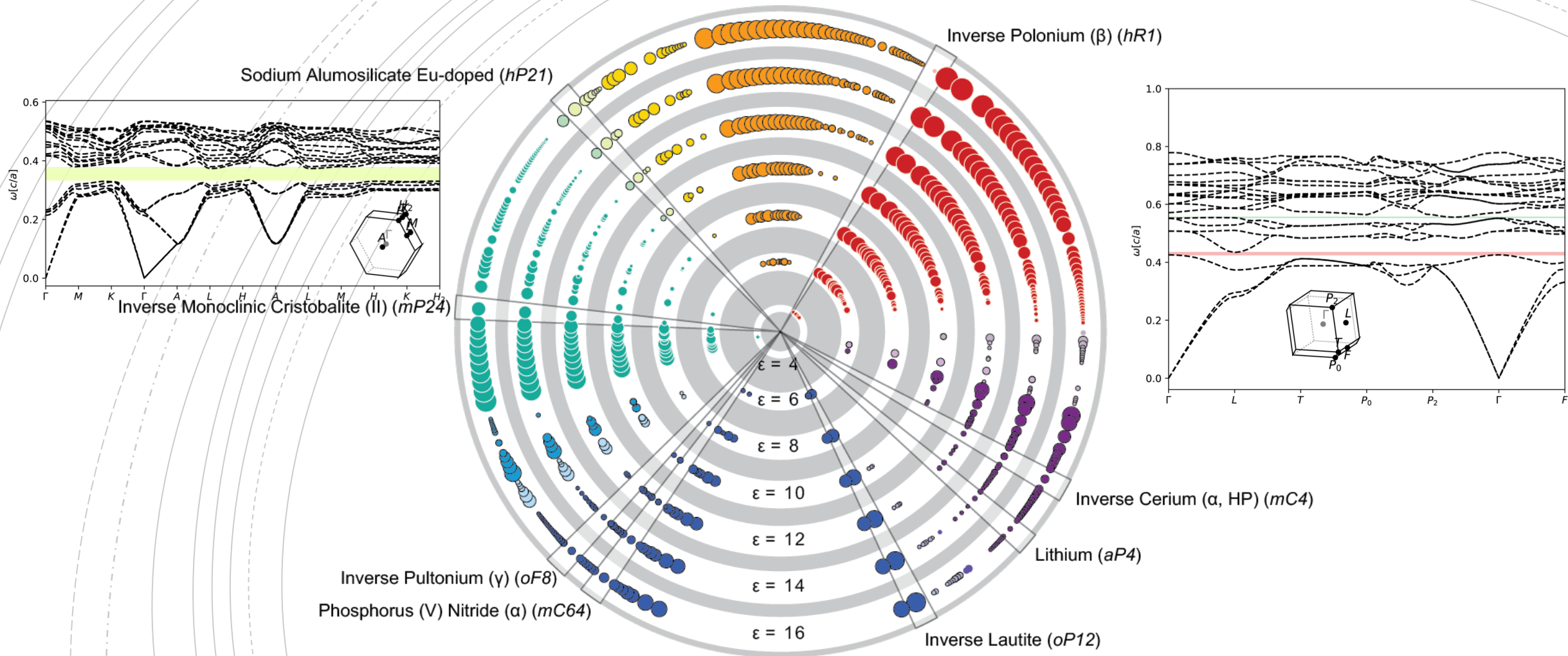


Inverse AB₁₃
 Maximum Gaps: 13.3% (Gaps 5-6),
 4.78% (Gaps 10-11)

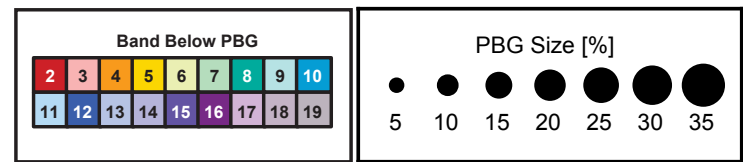


Each circle represents the maximum gap (circle size) found for a given template (radius), dielectric contrast (ring), and band location (color).

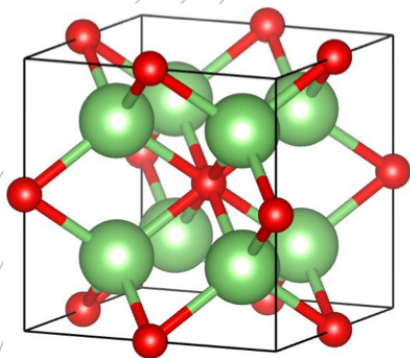
The diversity of three-dimensional photonic crystals
RKC, et al. Nature Communications 12,
<https://doi.org/10.1038/s41467-021-22809-6> (2021).



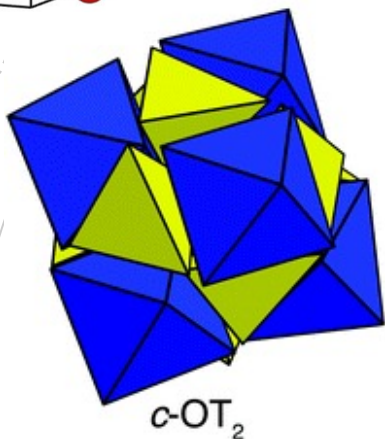
The diversity of three-dimensional photonic crystals
RKC, et al. *Nature Communications* 12,
<https://doi.org/10.1038/s41467-021-22809-6> (2021).



Each circle represents the maximum gap (circle size) found for a given template (radius), dielectric contrast (ring), and band location (color).



Lithium Oxide (cF12)



c-OT₂

Self-assembly of a space-tessellating structure in the binary system of hard tetrahedra and octahedra.

Cadotte, Andrew T., et al.

Soft matter 12.34 (2016): 7073-7078.

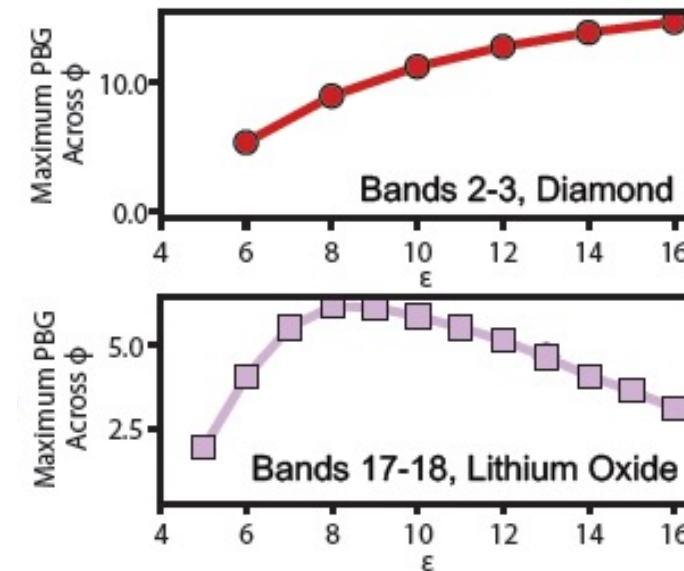
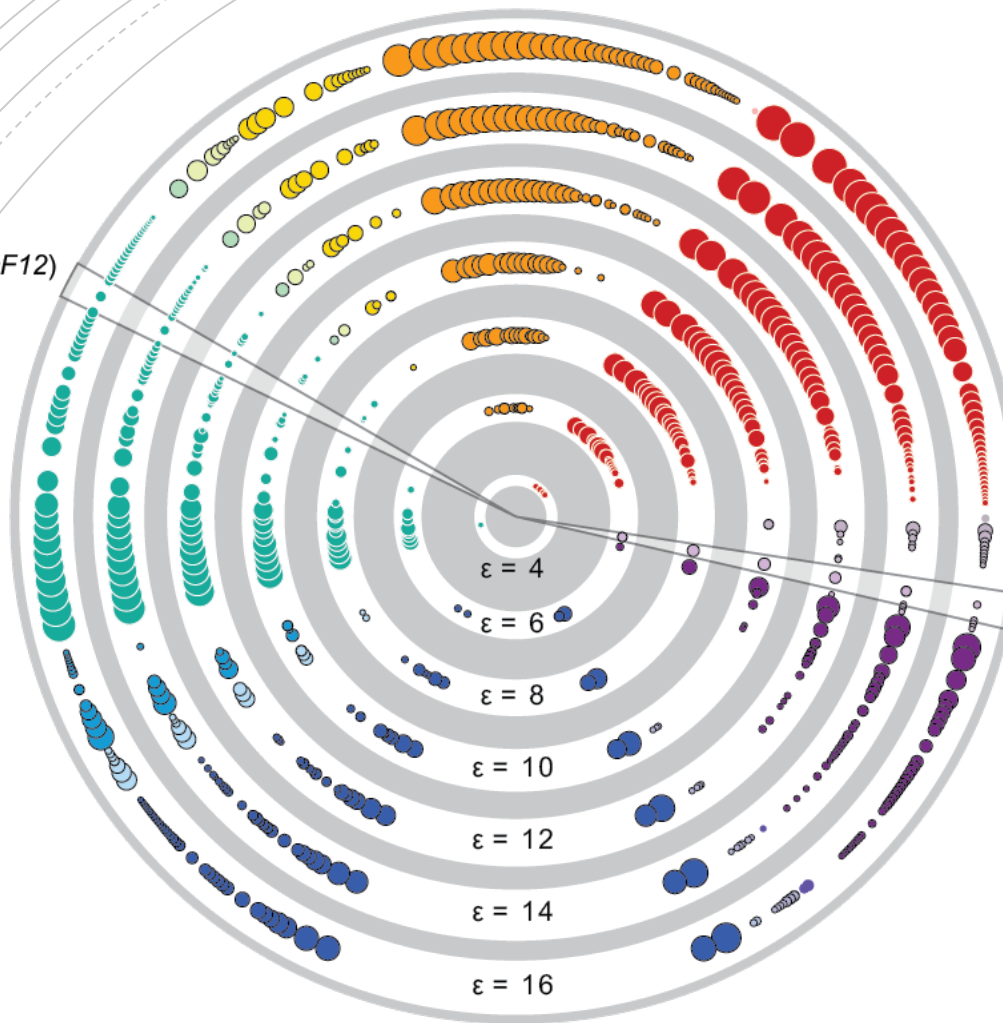
The diversity of three-dimensional photonic crystals

RKC, et al. *Nature Communications* 12, <https://doi.org/10.1038/s41467-021-22809-6> (2021).

For more detailed analysis, see SI Fig. 9.

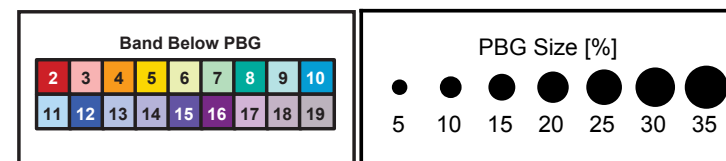
November 7, 2021

AICHe 2021



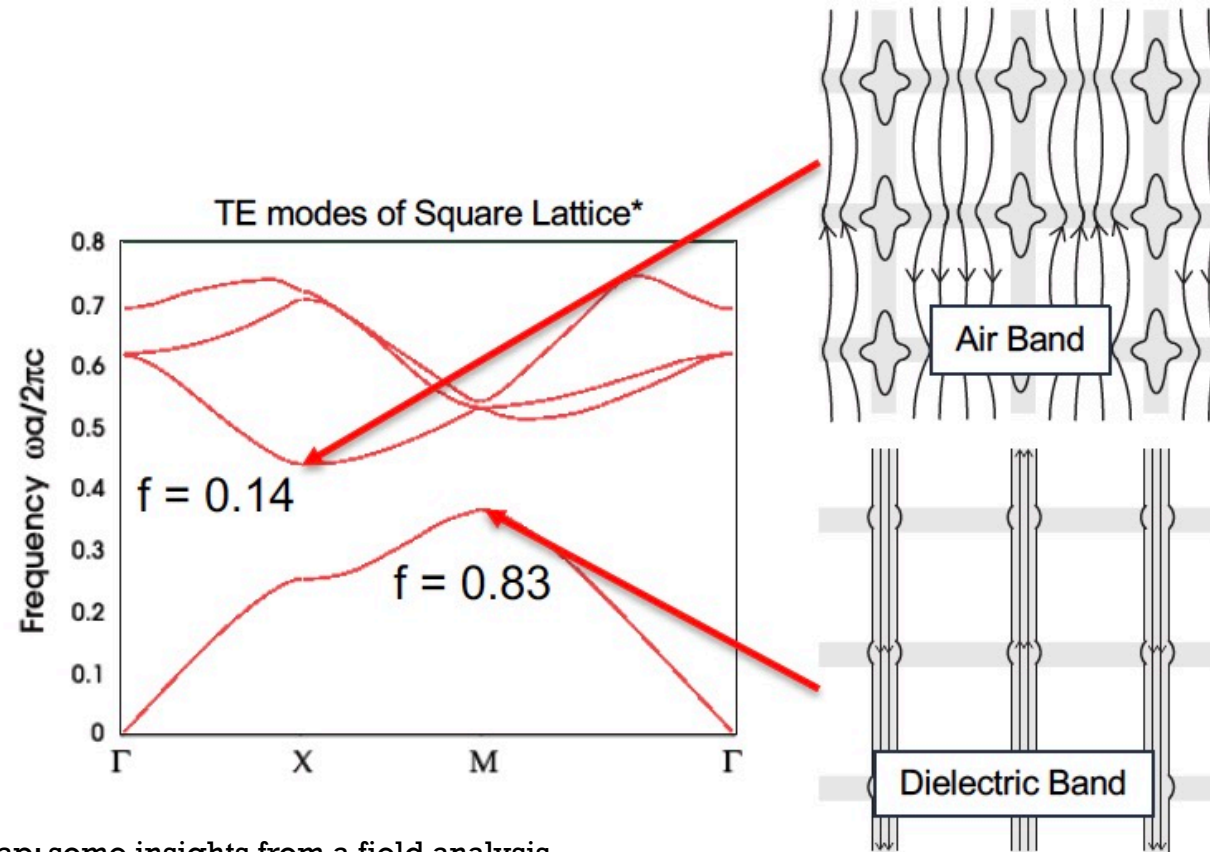
Lithium Oxide (cF12)

A band gap which is largest at intermediate dielectric constant has enormous potential for synthesis.



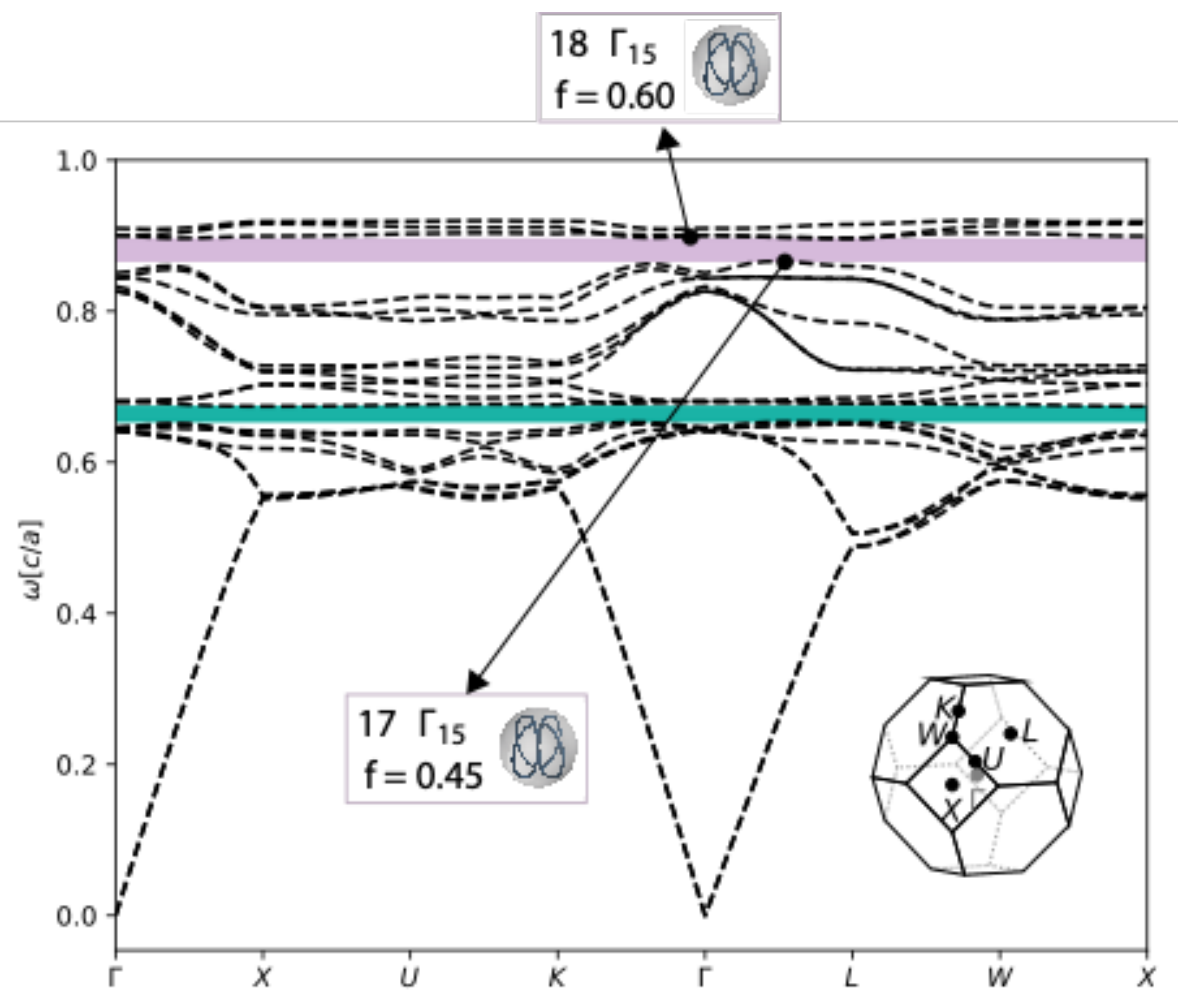
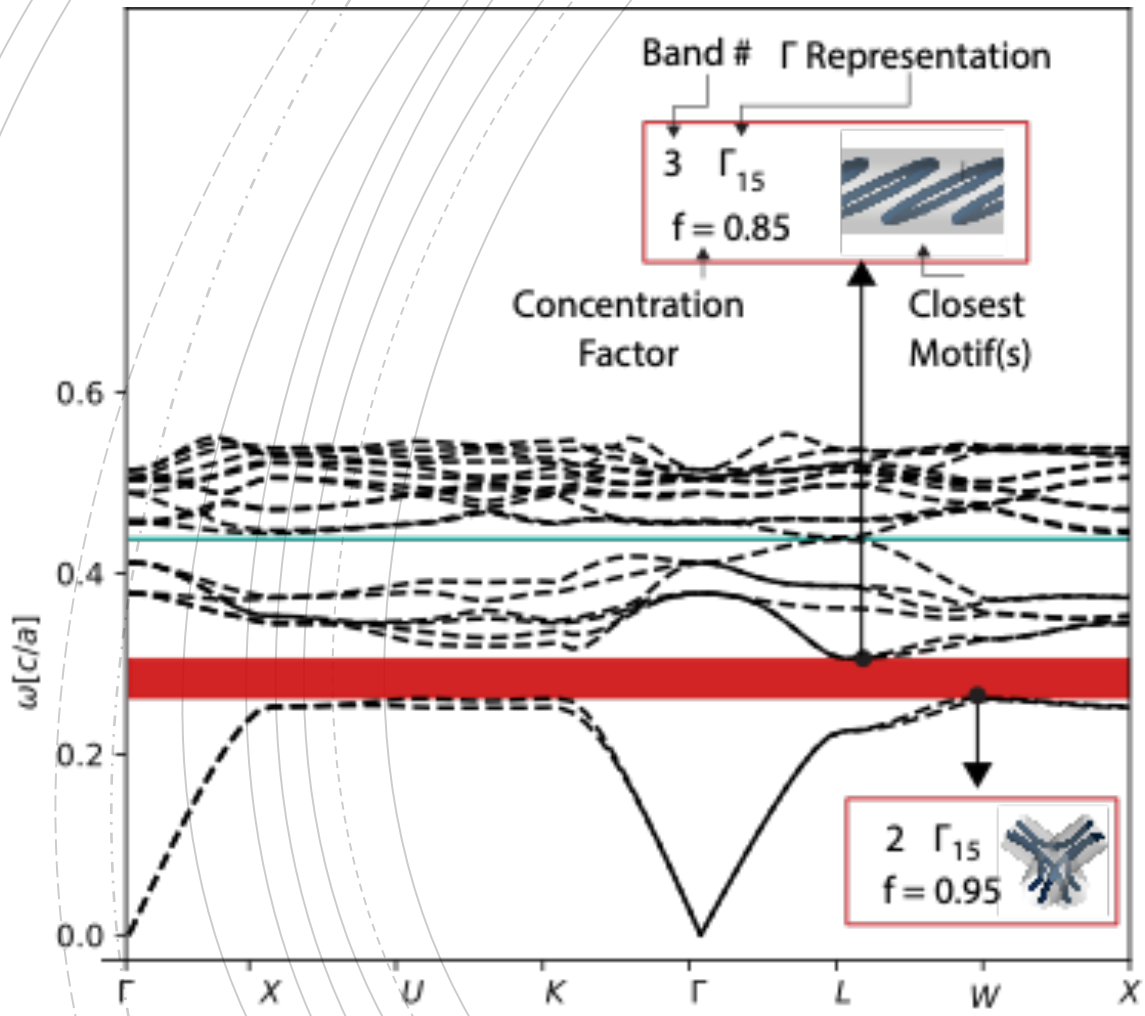
Each circle represents the maximum gap (circle size) found for a given template (radius), dielectric contrast (ring), and band location (color).

Conventional knowledge states that band gaps occur between bands of different localization of the energy density in either dielectric region.



Nature of the photonic band gap: some insights from a field analysis
R. D. Meade, A. M. Rappe, K. D. Brommer, and J. D. Joannopoulos
Journal of the Optical Society of America B (1993) 10 (2), pp. 328-332

Because the gap in lithium oxide does not occur between a “dielectric” and “air” band, the relationship between dielectric constant and gap size is similarly atypical.



Rose K. Cersonsky, James Antonaglia, Bradley Dice, Sharon C. Glotzer. Nature Communications 12 (2021)

Photonics Database: <https://glotzerlab.engin.umich.edu/photonics/index.html>

Appendix of Band Structures: <https://deepblue.lib.umich.edu/handle/2027.42/153520>

RK Cersonsky, J Dshemuchadse, J Antonaglia, G van Anders, SC Glotzer, Phys. Rev. Mat. 2, 125201 (2018).

RK Cersonsky, G van Anders, PM Dodd, SC Glotzer, PNAS 115, 1439–1444 (2018).

Y Zhou, RK Cersonsky, SC Glotzer, “A New Route to the Diamond Colloidal Crystal.”

Come see my other talks this week!

127b - The Search for Novel Mesoscale Materials

Monday, November 8, 2021

12:42 PM - 12:54 PM EDT

Marriott Copley Place - Salon A/B

203e - Improving Data Sub-Selection for Supervised Tasks with Principal Covariates Regression

Monday, November 8, 2021

4:30 PM - 4:45 PM EDT

Marriott Copley Place - Salon H/I

The Diversity of Three-Dimensional Photonic Crystals for Colloidal Self-assembly

