Division of Colloid and Surface Chemistry
American Chemical Society

2021 Victor K. LaMer Award

Dr. Rose Cersonsky (currently Postdoctoral Research at EPFL)

- B.S. 2014 in Materials Science and Engineering, University of Connecticut
- Ph.D. 2019 in Macromolecular Science and Engineering, University of Michigan
    - Advisor: Sharon Glotzer
- Postdoctoral Associate, EPFL, 2019-present

Dissertation: "Designing Particle Shapes for Self-Assembly of Novel Colloidal Crystals"

Ph.D. research accomplishments:

- Published 6 papers (5 as first author), including 2 focused on education
- Developed fundamental understanding of the role of particle shape, excluded volume and entropic packing in controlling symmetry of ordered colloidal assemblies. Pioneered data-driven approaches to predicting and understanding structure-property relations in ordered colloidal phases, including photonics.

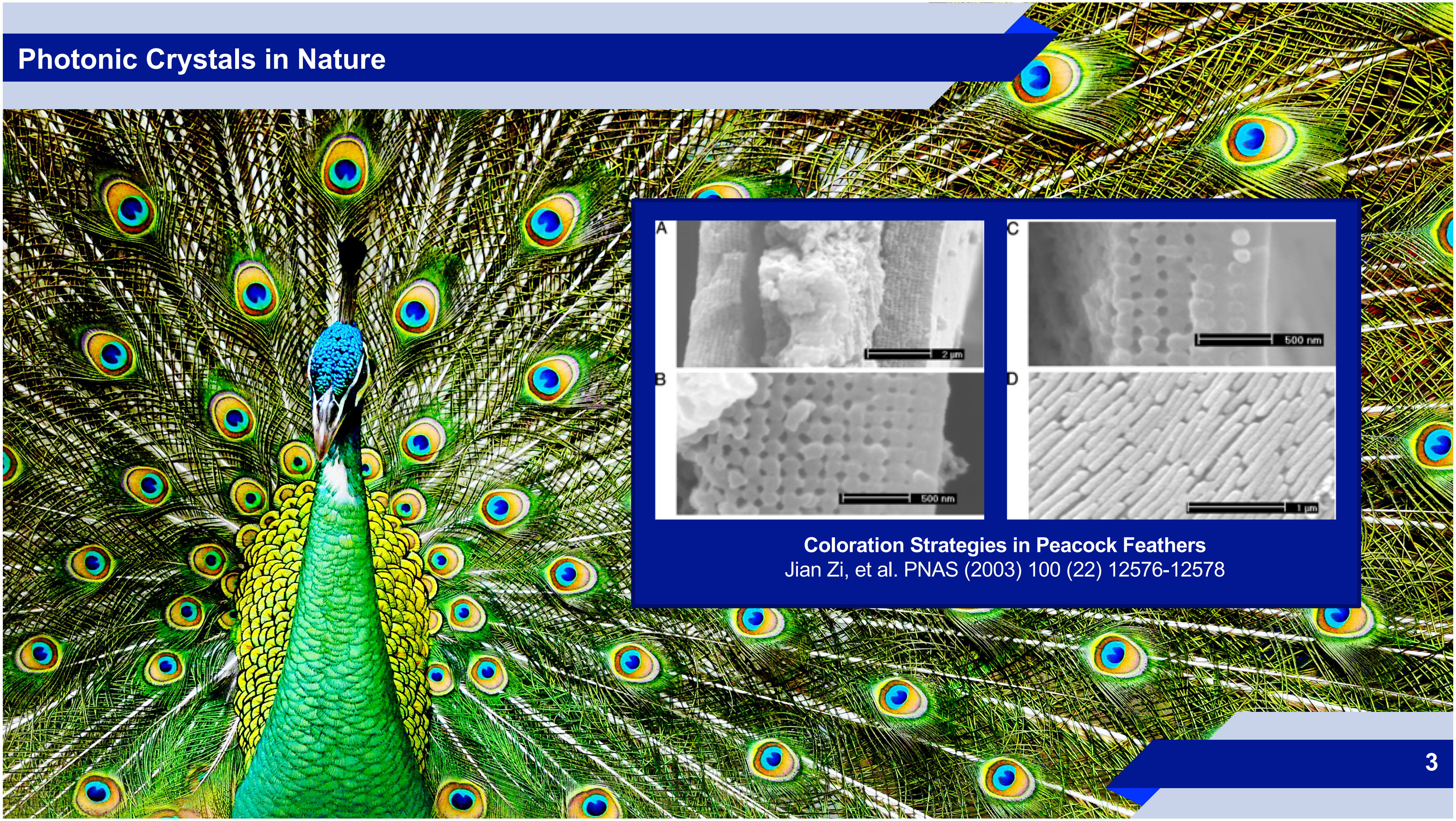
Selection committee:

Matthew Helgeson (chair), University of California Santa Barbara
Brandi Cossairt, University of Washington
Kyle Bishop, Columbia University
Maria Santore, University of Massachusetts Amherst

Designing Nanoparticles for Self-Assembly of Novel (Photonic) Materials

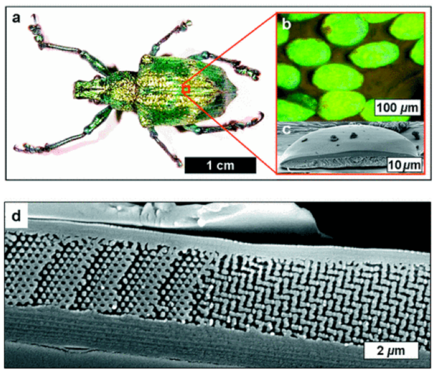
Dr. Rose K. Cersonsky[1,*]

[1]Macromolecular Science and Engineering, University of Michigan, Ann Arbor, Michigan
[*]Laboratory of Computational Science and Modeling, EPFL, Switzerland

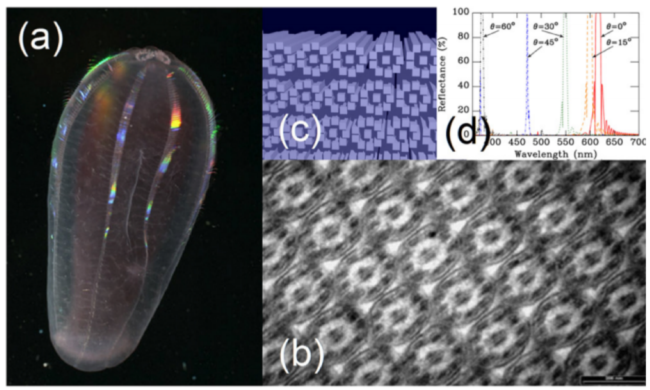


Coloration Strategies in Peacock Feathers
Jian Zi, et al. PNAS (2003) 100 (22) 12576-12578

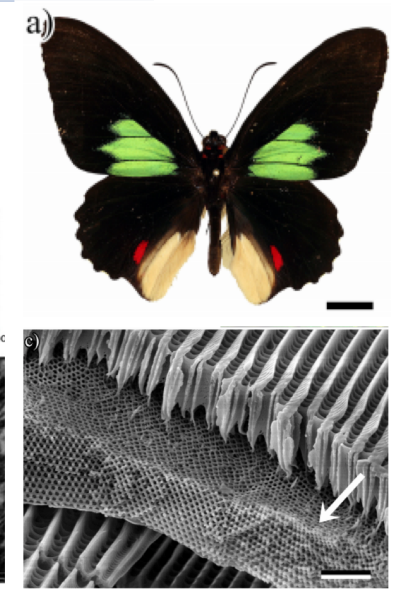
Photonic Crystals in Nature



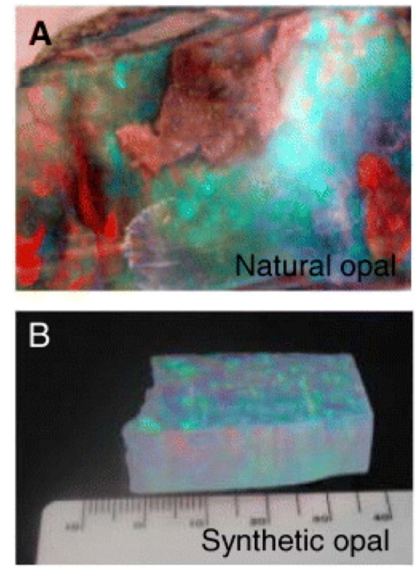
Discovery of a diamond-based photonic crystal structure in beetle scales
Jeremy W. Galusha*, et al.*
Phys. Rev. E 77, 050904



Optical properties of the iridescent organ of the comb-jellyfish Beroë cucumis (Ctenophora)
Victoria Welch, *et al.*
Phys. Rev. E 73, 041916 2006



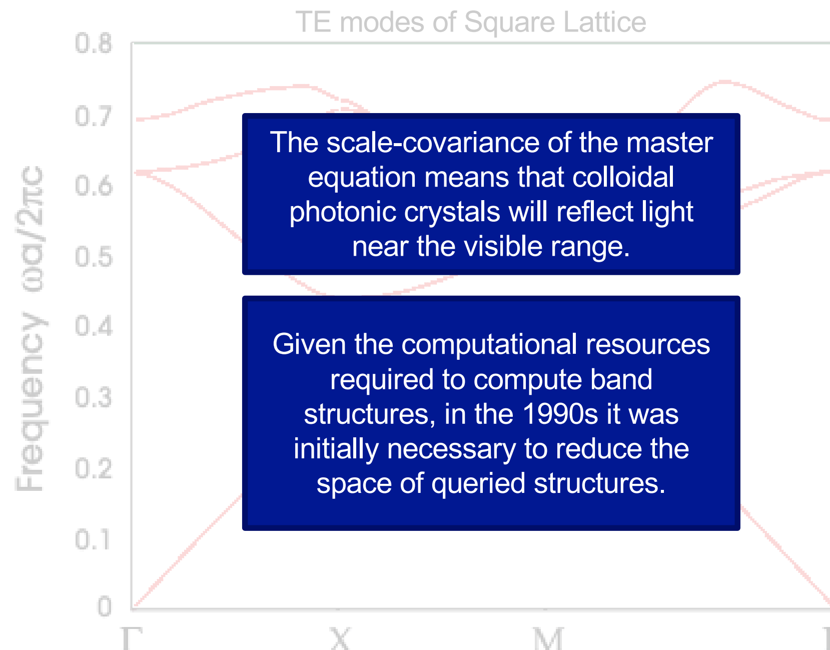
Optical properties of gyroid structured materials: from photonic crystals to metamaterials
James A. Dolan , *et al.*
Advanced Optical Materials 3 (1), 12-32



Tunable structural color in organisms and photonic materials for design of bioinspired materials
Hiroshi Fudouzi
Sci. Technol. Adv. Mater. (2011) 12 064704

The Physics of Photonic Crystals

$$\nabla\times\left(\frac{1}{\boxed{\varepsilon(\mathbf{r})}}\nabla\times\mathbf{H}(\mathbf{r})\right)=\frac{\boxed{\omega^2}}{c^2}\mathbf{H}(\mathbf{r})$$



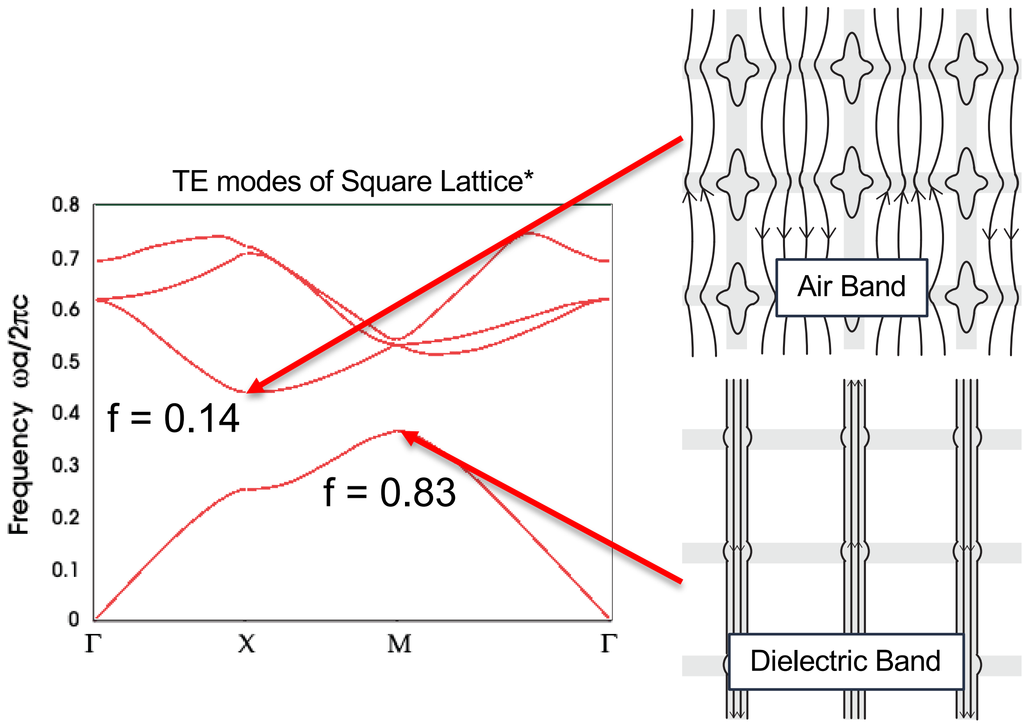
The scale-covariance of the master equation means that colloidal photonic crystals will reflect light near the visible range.

Given the computational resources required to compute band structures, in the 1990s it was initially necessary to reduce the space of queried structures.

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

Derivation of Master Equation:
Joannopoulos (2008)

Field Analysis of Photonic Crystals



$$f = \frac{\int_{V_\varepsilon} \mathbf{E}^*(\mathbf{r}) \cdot \mathbf{D}(\mathbf{r})d\mathbf{r}}{\int \mathbf{E}^*(\mathbf{r}) \cdot \mathbf{D}(\mathbf{r})d\mathbf{r}}$$

Nature of the photonic band gap: some insights from a field analysis
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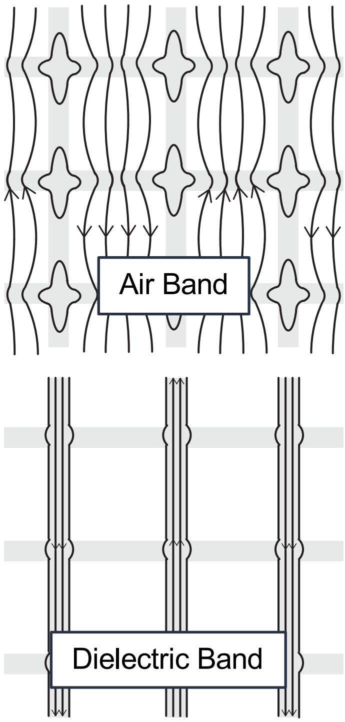
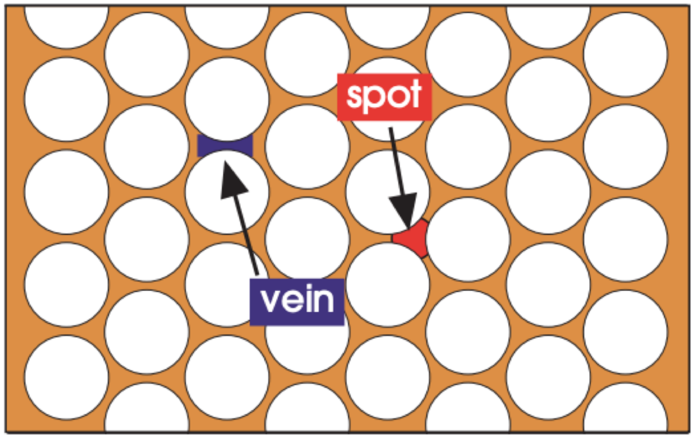
*One can conduct similar analysis for the transverse magnetic (TM) polarization.

Field Analysis of Photonic Crystals



Photonic band gaps emerge when there is a clear “dielectric” band and “air” band.

Electric energy can localize more easily in the high dielectric medium when it forms a **connected network** with regions of **relative isolation**.

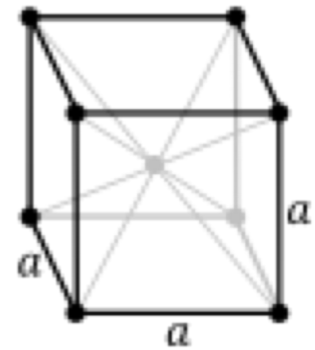


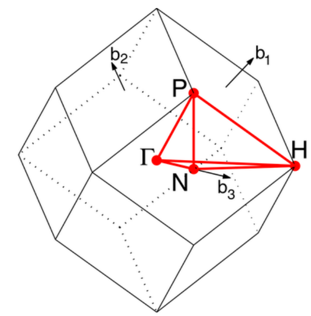
Nature of the photonic band gap: some insights from a field analysis
R. D. Meade, A. M. Rappe, K. D. Brommer, and J. D. Joannopoulos
Journal of the Optical Society of America B (1993) 10 (2), pp. 328-332

Design Rules for Photonic Crystals

The largest PBG will occur in lattices with the most spherical Brillouin zones.

Body-Centered Cubic

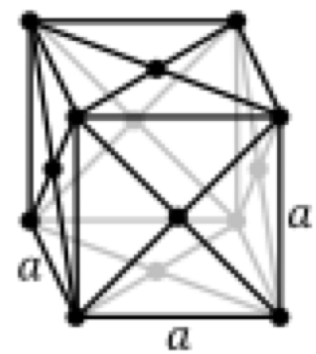


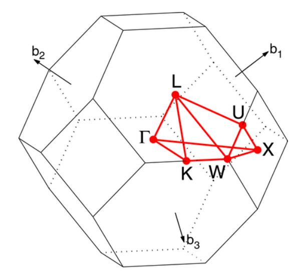


BCC path: Γ-H-N-Γ-P-H|P-N

[Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]

Face-Centered Cubic



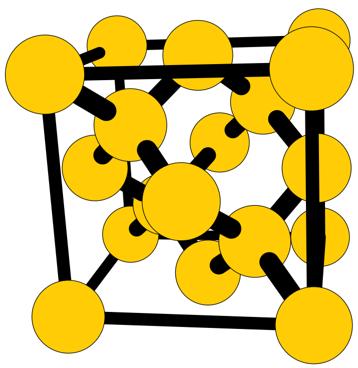


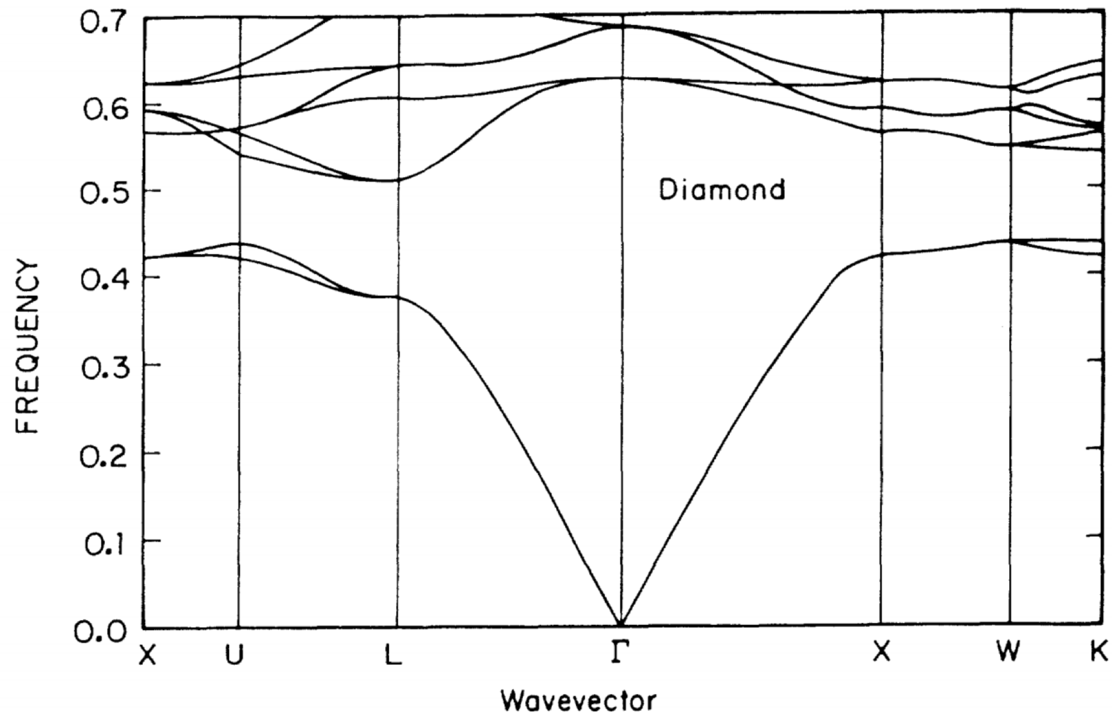
FCC path: Γ-X-W-K-Γ-L-U-W-L-K|U-X

[Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]

Images from:
wikipedia.org

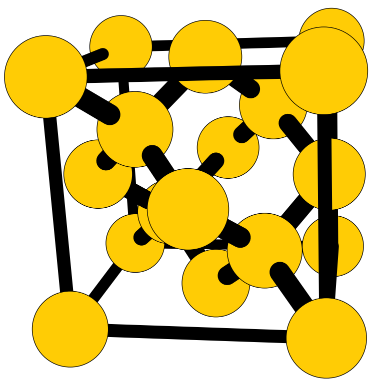
Synthesizing Photonic Crystals



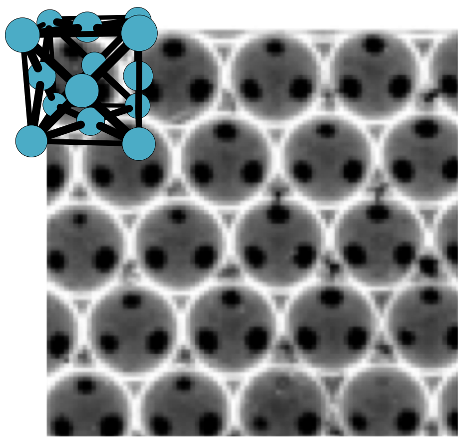


Existence of a Photonic Gap in Periodic Dielectric Structures
K. M. Ho, C. T. Chan, and C. M. Soukoulis
Physics Review Letters 65, 25 (1990)

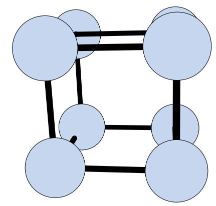
Synthesizing Photonic Crystals



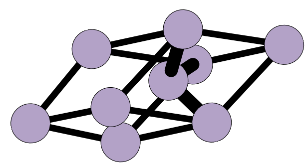
Diamond
(Ho, Chan, and Soukolis, 1990)



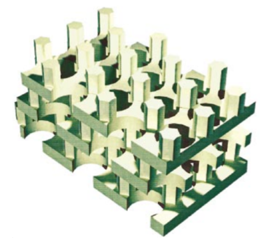
Inverse Opal/FCC
(Sözüer, et al., 1993)



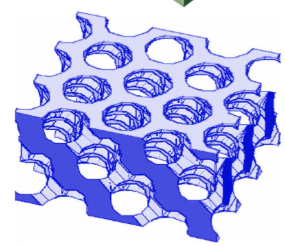
Simple Cubic
(Sözüer and Haus, 1993)



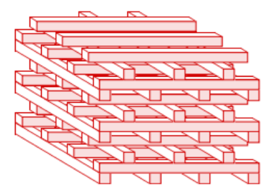
A7
(Chan, et al., 1994)



Layer-by-Layer
(incl. Johnson and Joannopoulos, 2000)

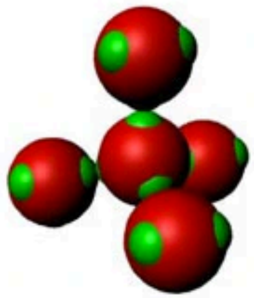


Yablonovite
(Yablonovitch, et al., 1991)

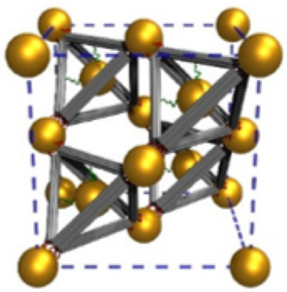


Woodpile
(Ho, et al., 1994)

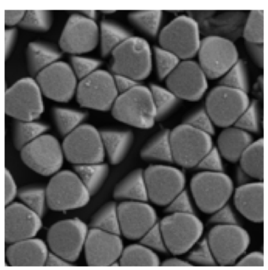
Synthesizing Photonic Crystals



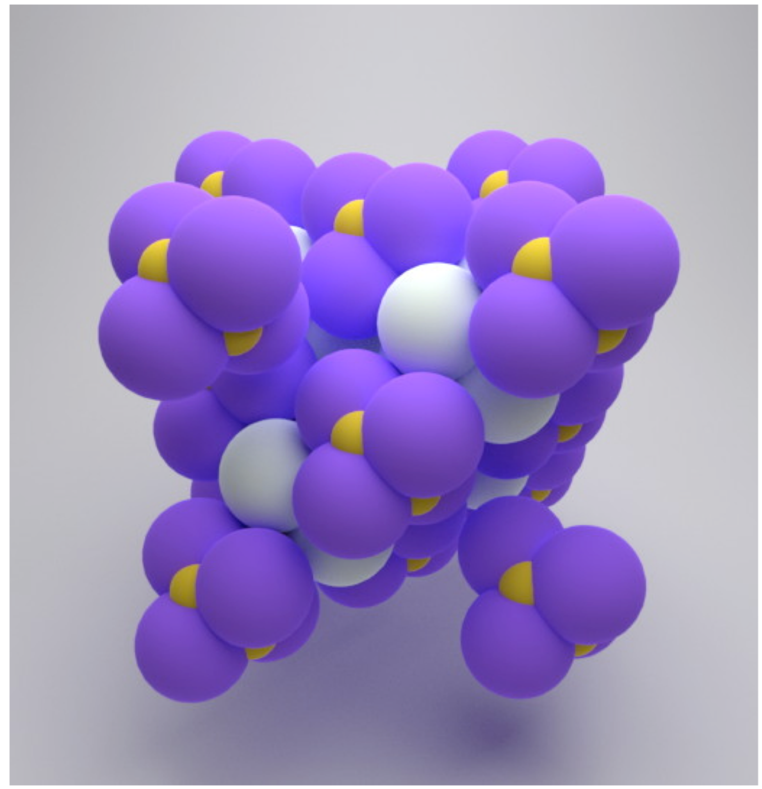
Colloidal crystals with diamond symmetry at optical lengthscales
Yifan Wang, et al.
Nature Comm. 8, 14173 (2017)



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

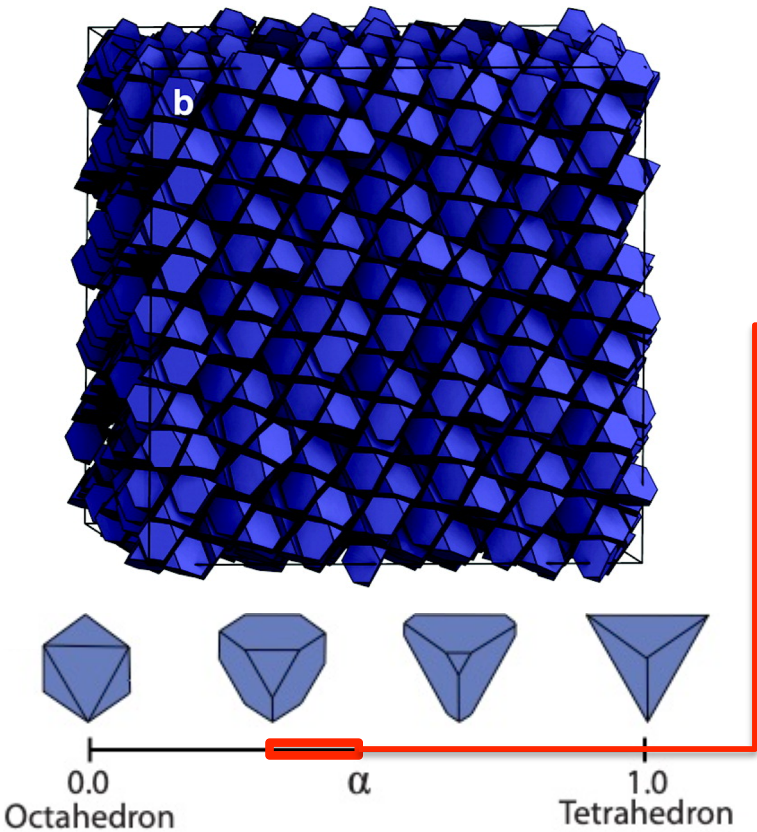


Entropy driven assembly of truncated colloidal tetrahedra into diamond structure
Zhe Gong, et al.

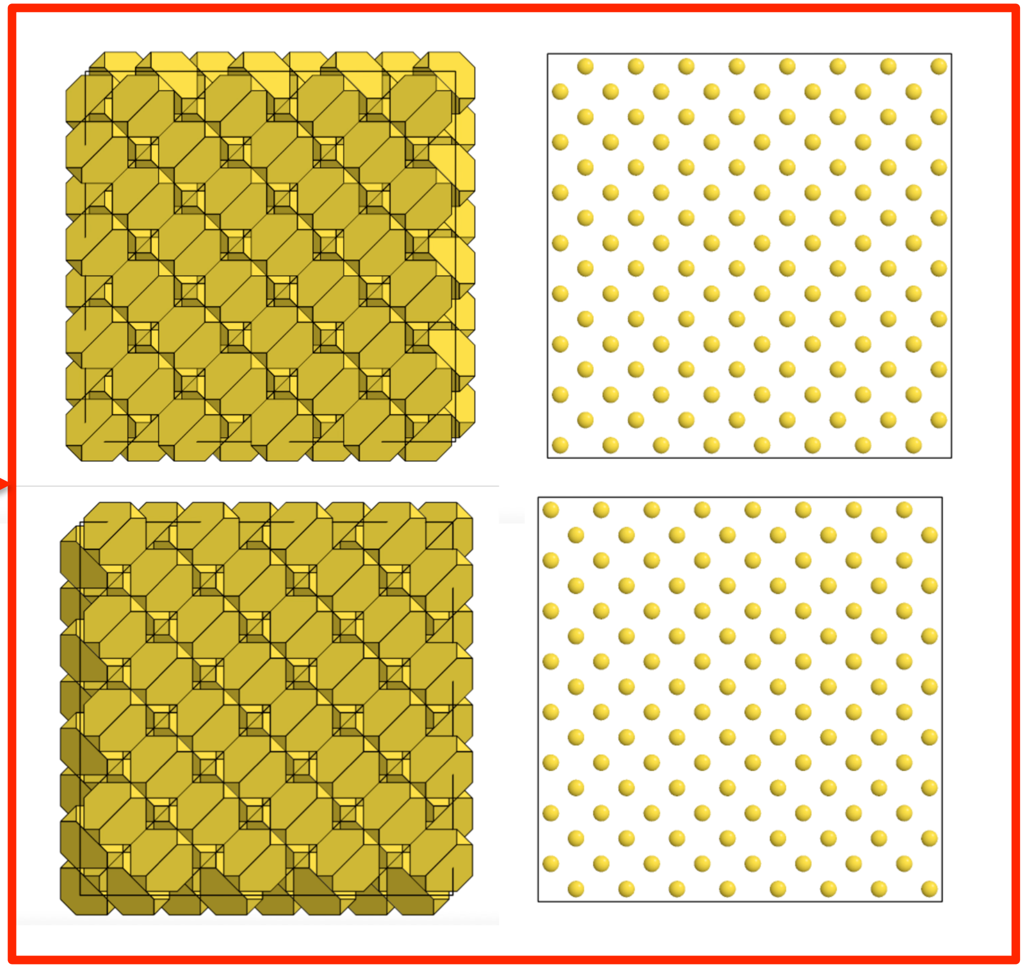


Colloidal diamond
He, M., et al.
Nature 585, 524–529 (2020).

Synthesizing Photonic Crystals

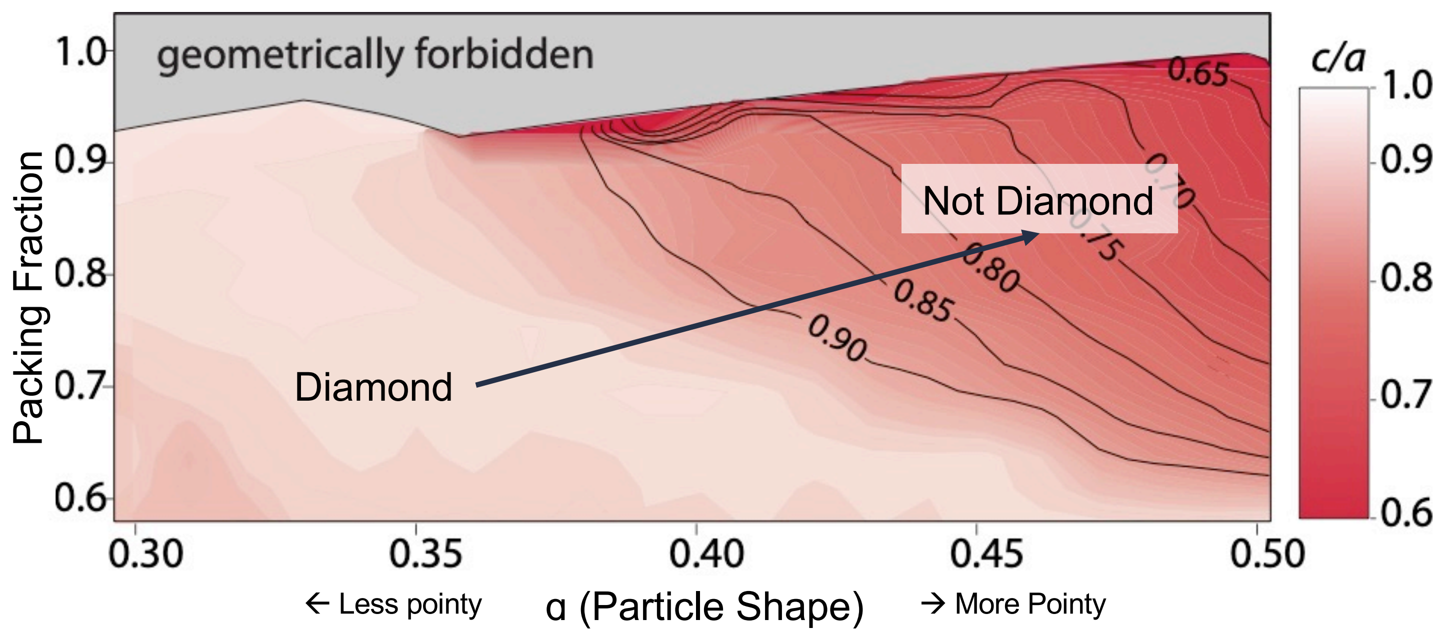


Crystalline Assemblies and Densest Packings of a Family of Truncated Tetrahedra & the Role of Directional Entropic Forces
Pablo F. Damasceno, et al.ACS Nano, 2012, 6 (1), pp 609–614



Pressure-tunable photonic band gaps in an entropic colloidal crystal
RKC, et al. Physical Review Materials (2018) 2(12), 125201.

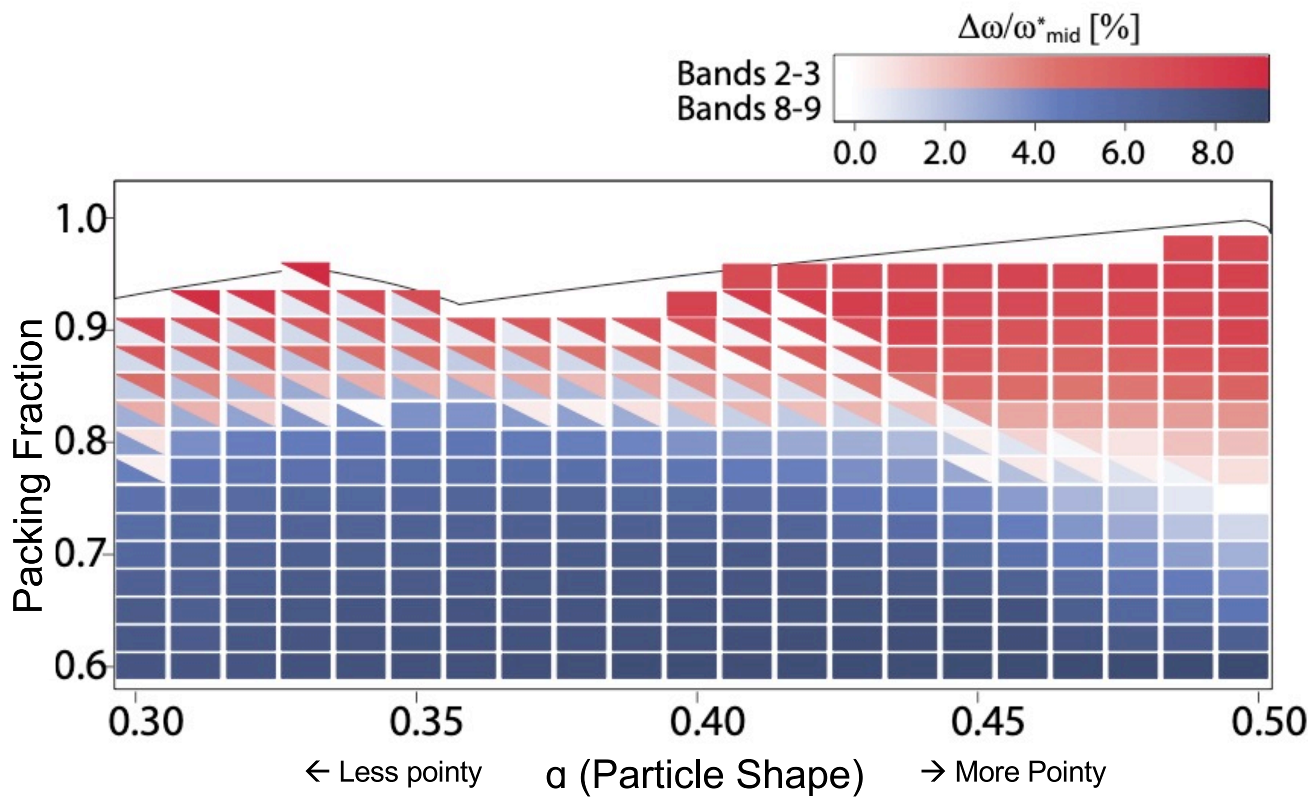
Synthesizing Photonic Crystals



Many diamond-assembling nanoparticles will transition to a tetragonal derivative with increased pressure.

Pressure-tunable photonic band gaps in an entropic colloidal crystal
RKC, et al. Physical Review Materials (2018) 2(12), 125201.

Synthesizing Photonic Crystals



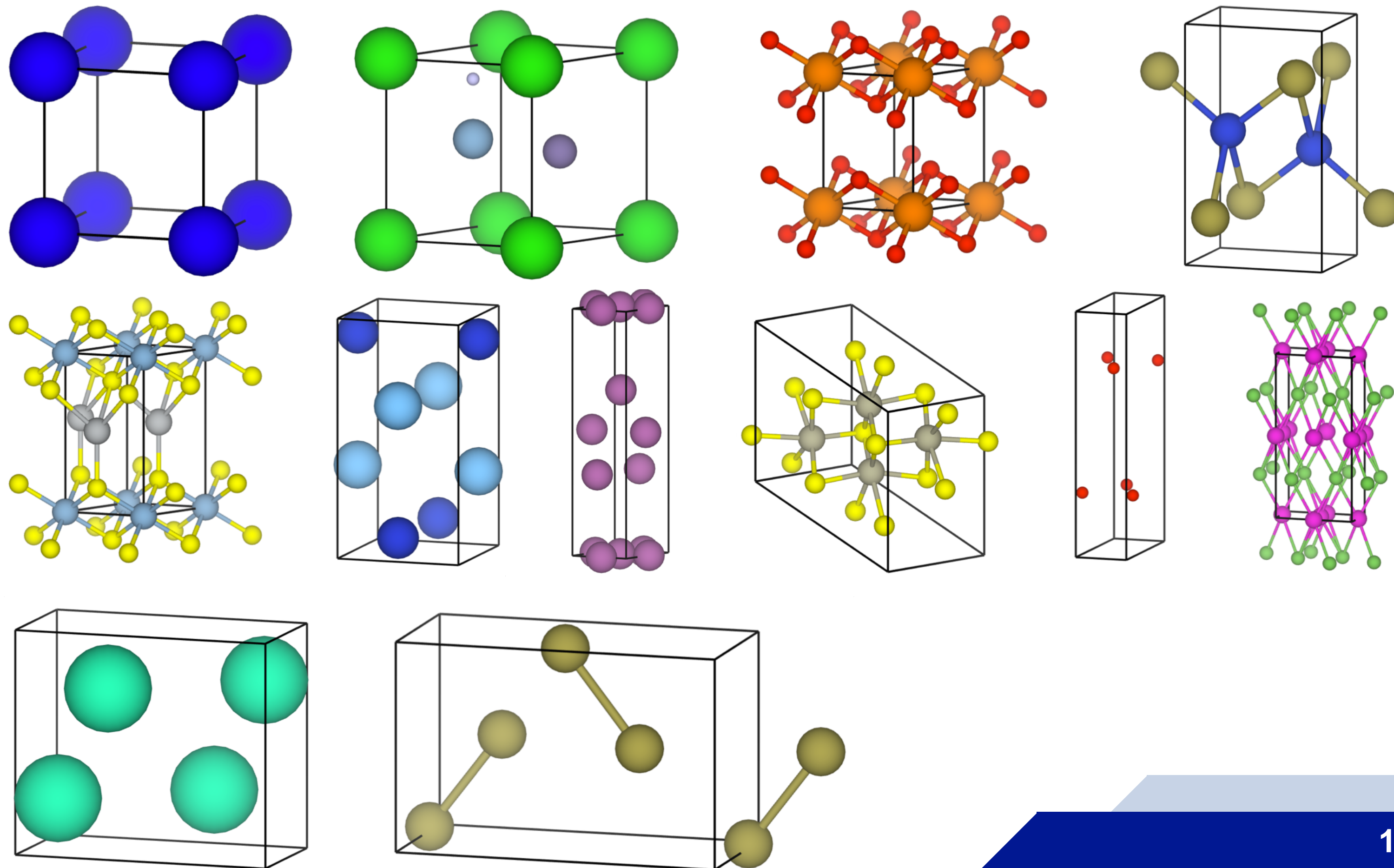
Many diamond-assembling nanoparticles will transition to a tetragonal derivative with increased pressure.

This symmetry reduction does not close the photonic band gaps, and with these particles a multi-state material is possible.

Pressure-tunable photonic band gaps in an entropic colloidal crystal
RKC, et al. Physical Review Materials (2018) 2(12), 125201.

What are the span of crystal structures capable of supporting a photonic band gap?

Calculating Photonic Band Structures



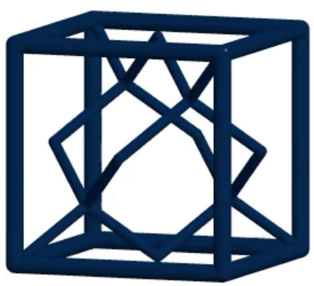
ICSD

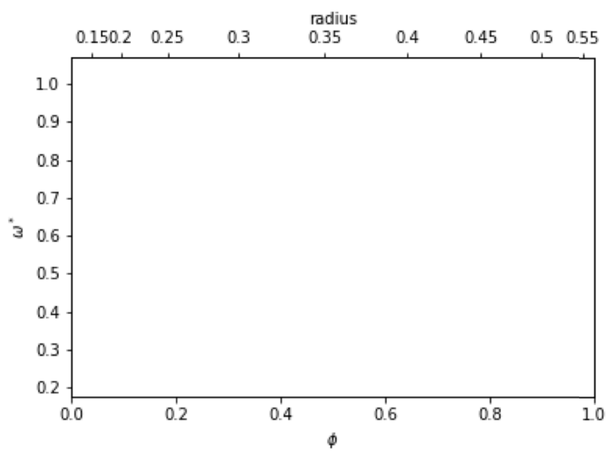
FIZ Karlsruhe

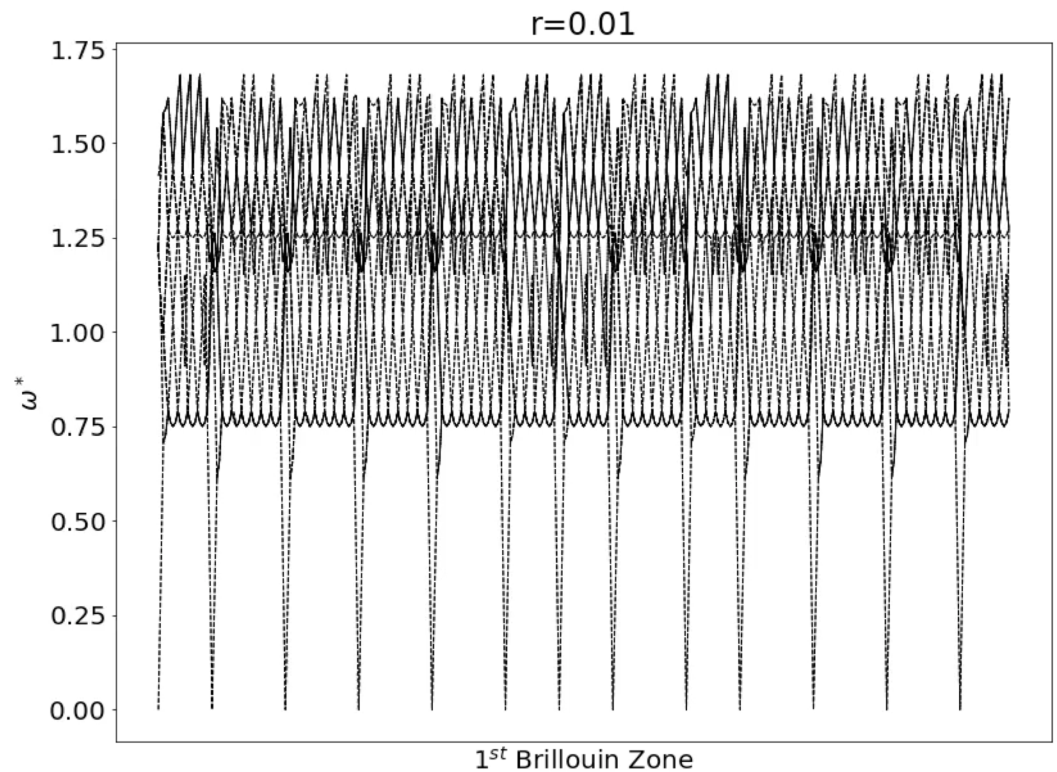
COD

Calculating Photonic Band Structures

MIT Photonic-Bands

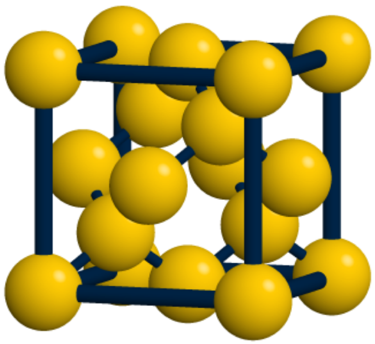


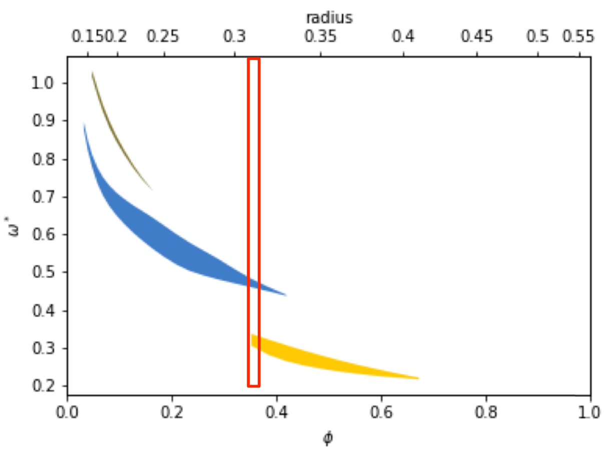


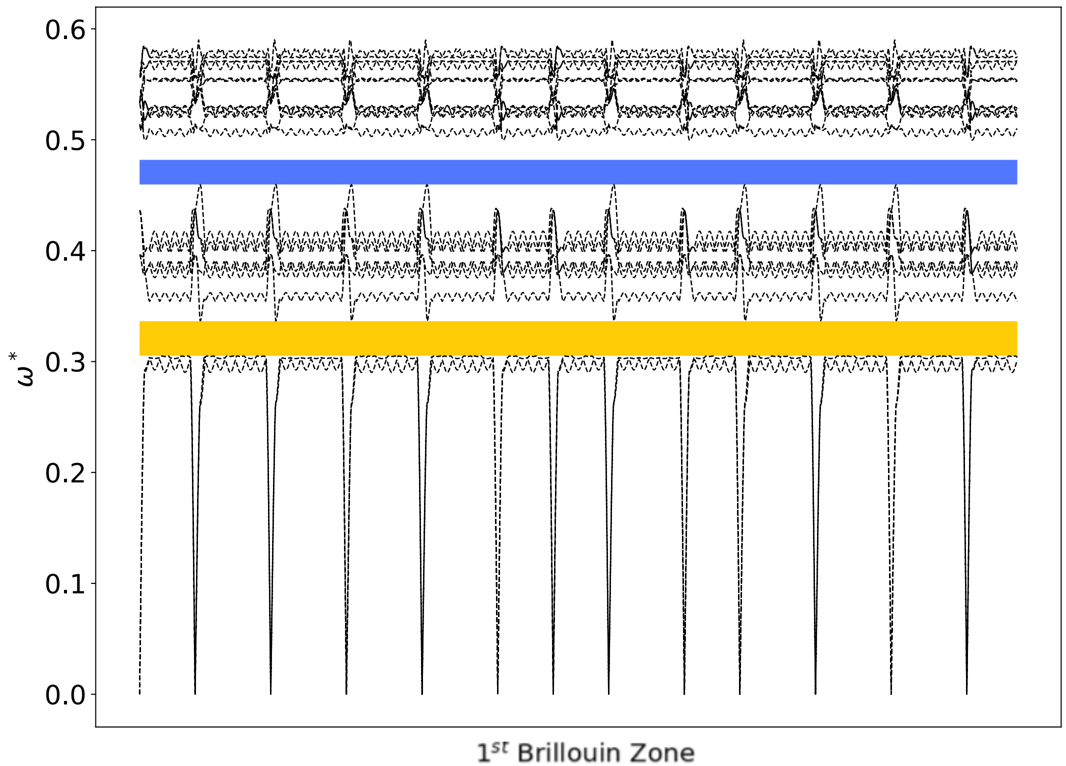


The diversity of three-dimensional photonic crystals
RKC, et al. *Nature Communications* 12, https://doi.org/10. 1038/s41467-021-22809-6 (2021).

Calculating Photonic Band Structures







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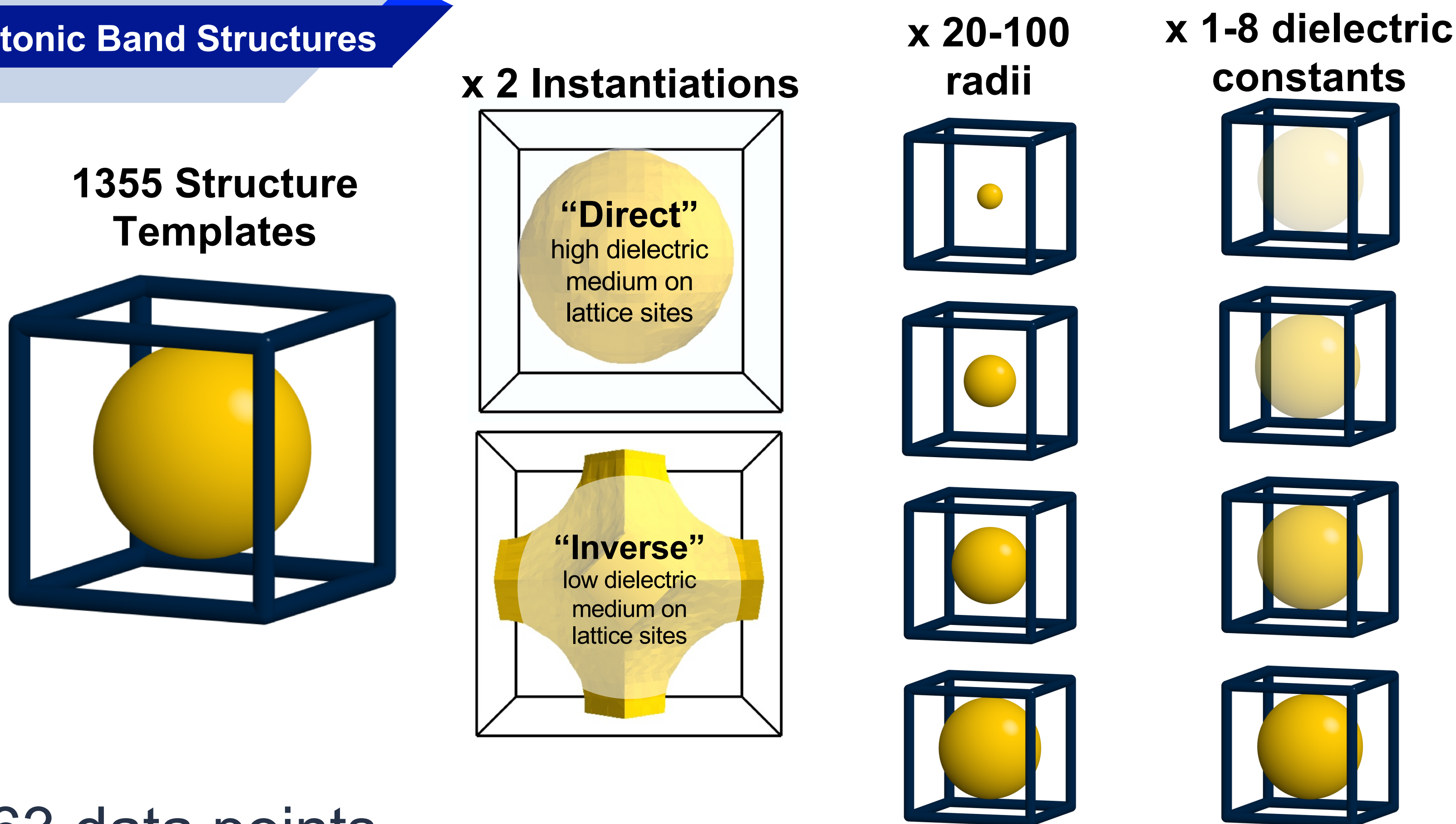

=151,163 data points

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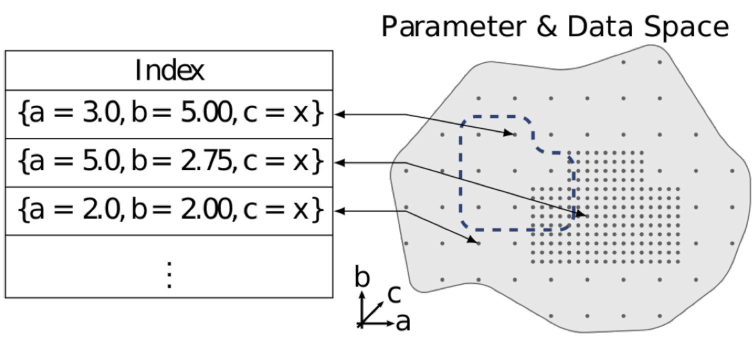
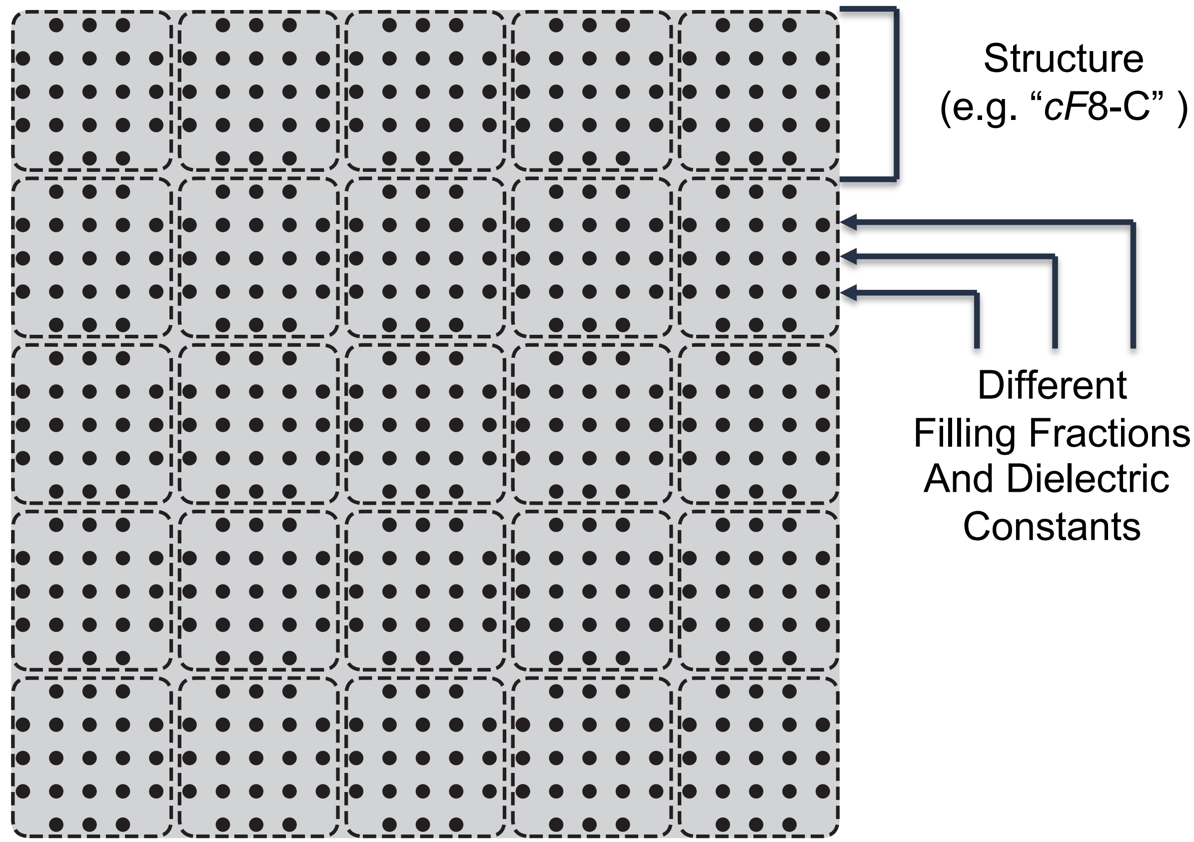
RKC, et al. *Nature Communications* 12, https://doi.org/10. 1038/s41467-021-22809-6 (2021).

Calculating Photonic Band Structures



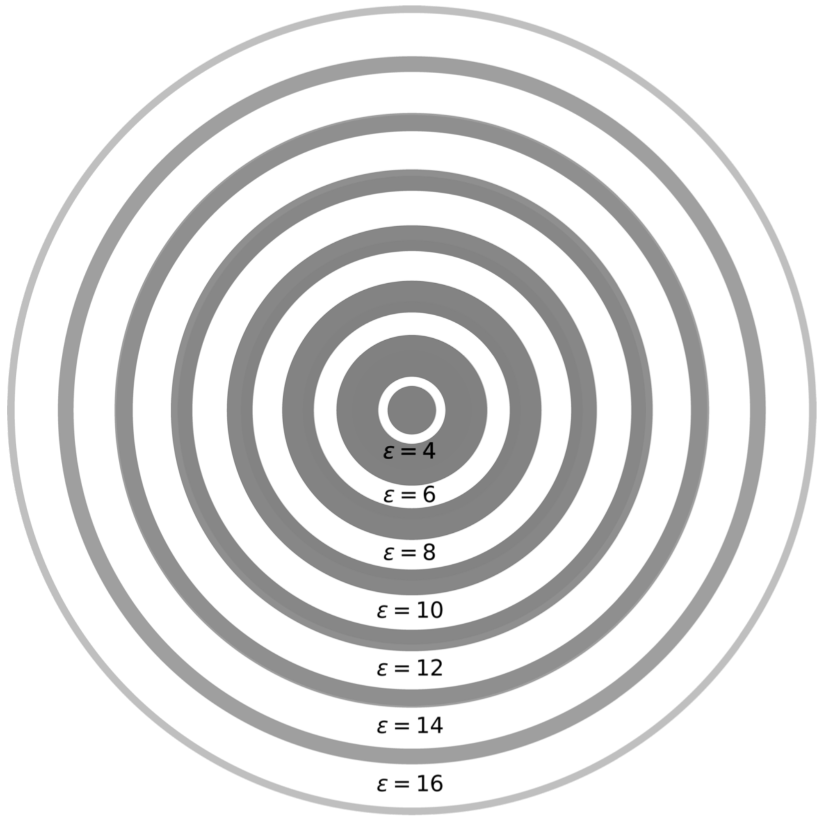
signac.io

Photonics Dataspace



Simple data and workflow management with the signac framework
C. S. Adorf, P. M. Dodd, V. Ramasubramani, and S. C. Glotzer, (2018) Comput. Mater. Sci., 146(C):220-229, doi:10.1016/j.commatsci.2018.01.035.

Results



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).

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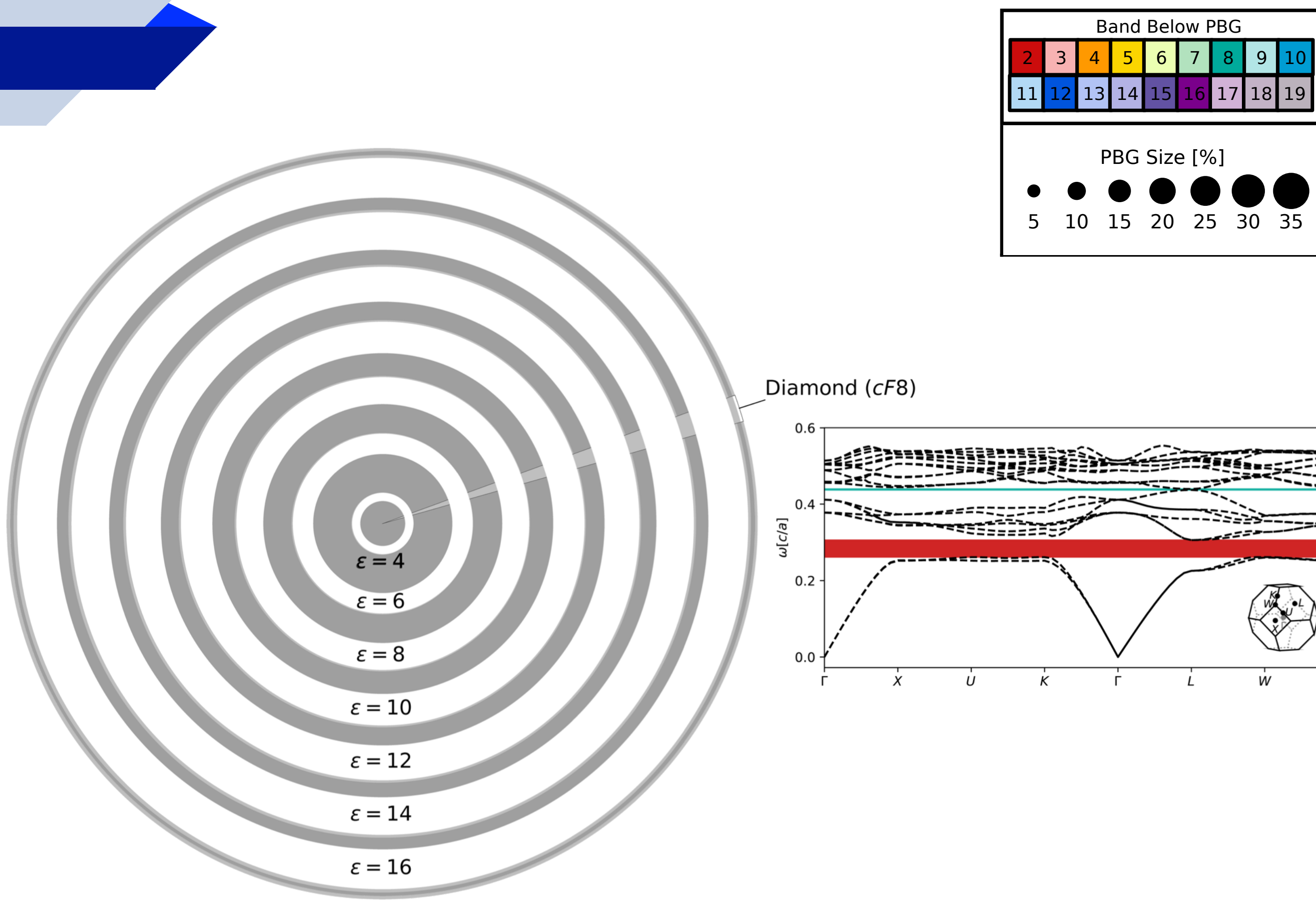

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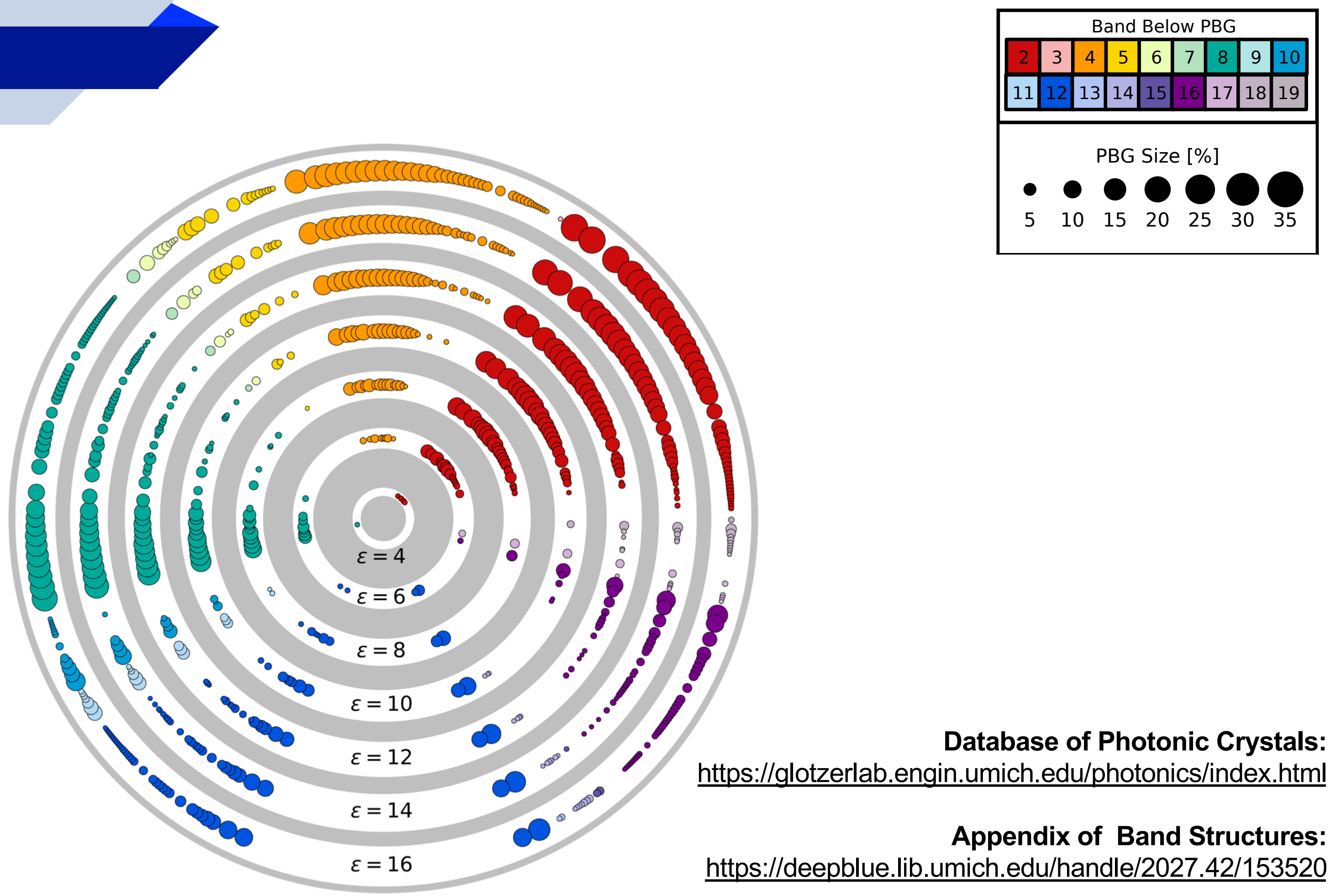

Database of Photonic Crystals:
https://glotzerlab.engin.umich.edu/photonics/index.html

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

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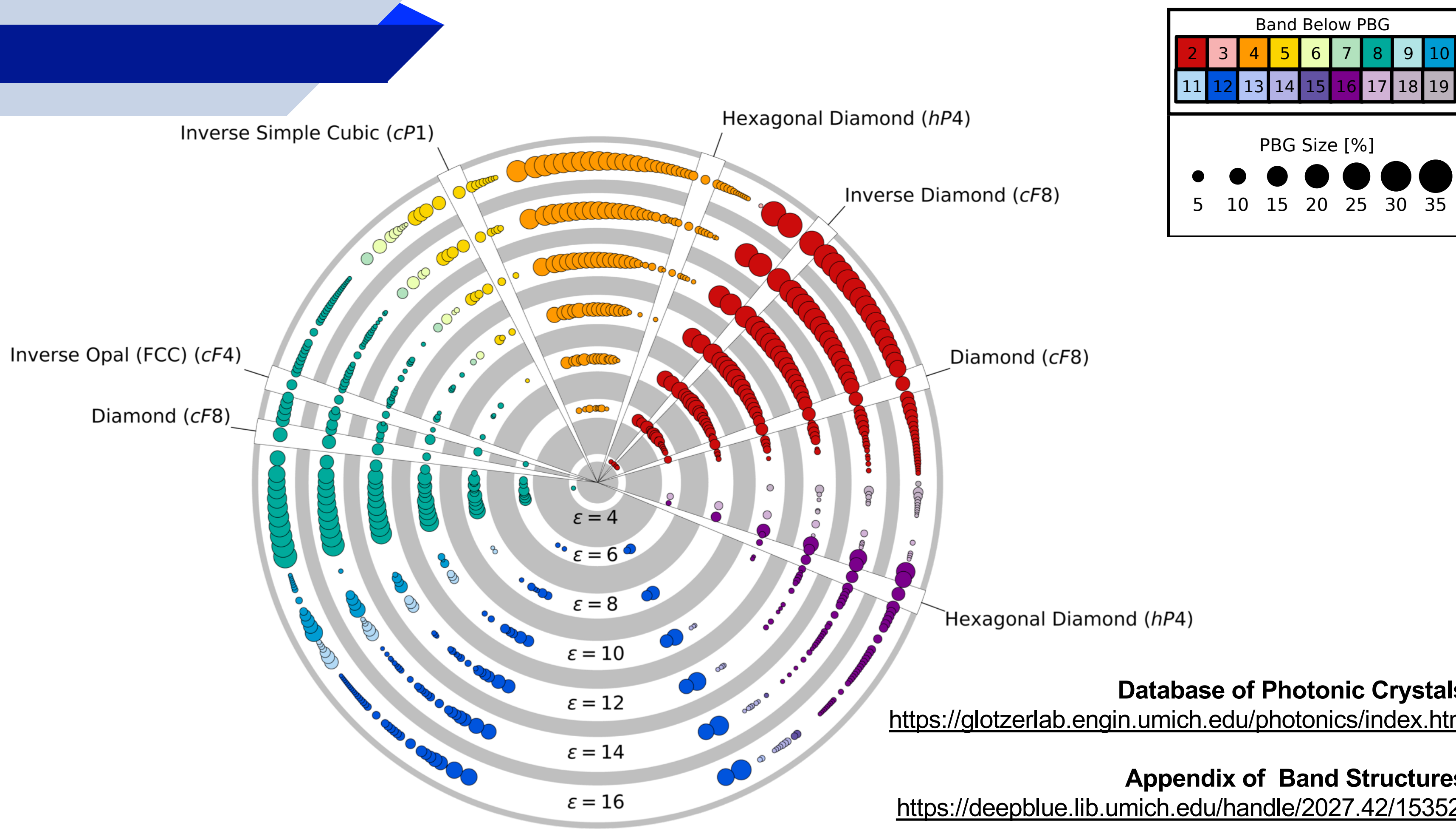

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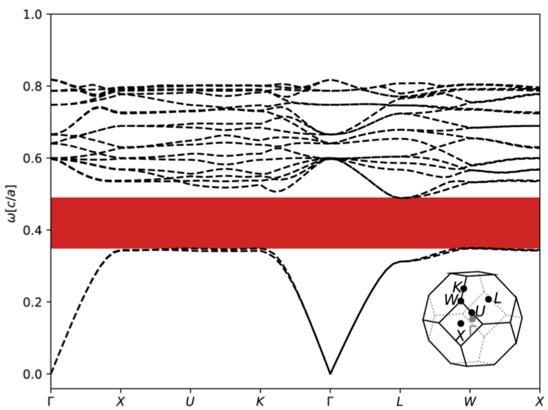
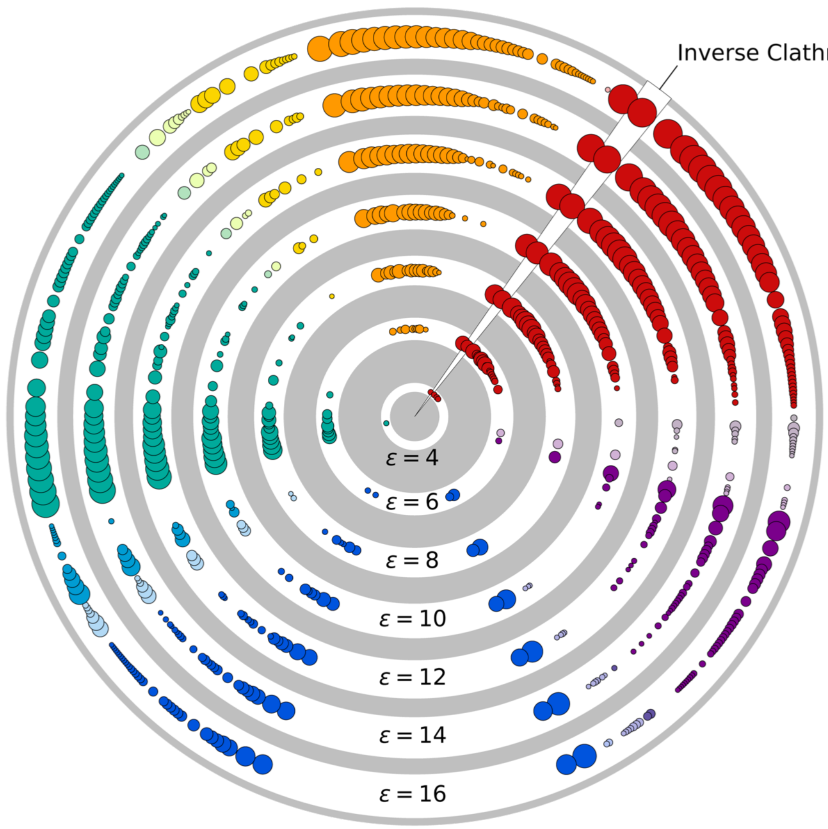
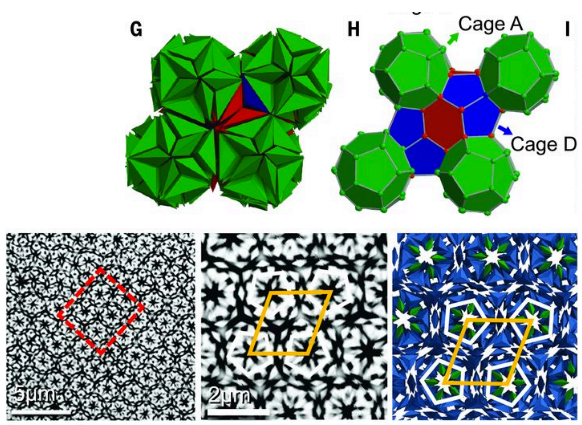
Results

Inverse Clathrate-II







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).

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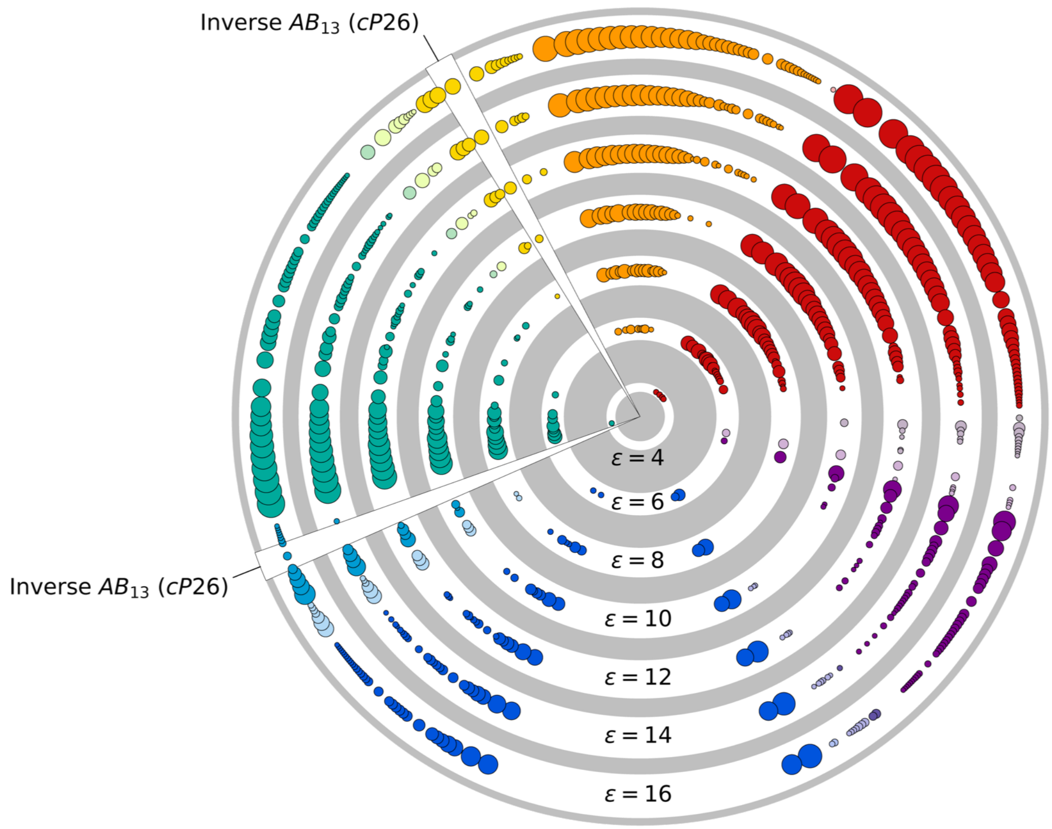

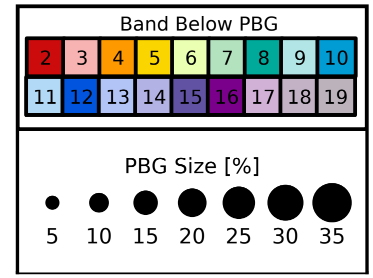

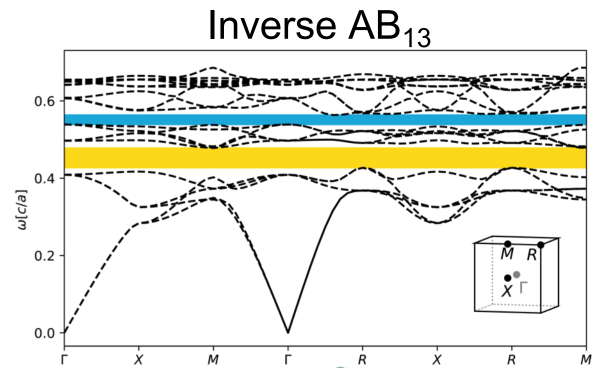

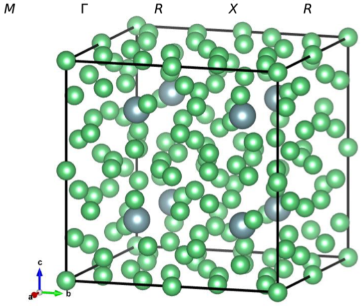

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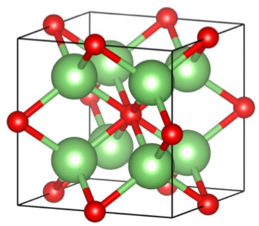
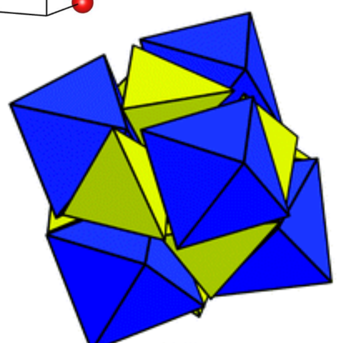
RKC, et al. *Nature Communications* 12, https://doi.org/10. 1038/s41467-021-22809-6 (2021).

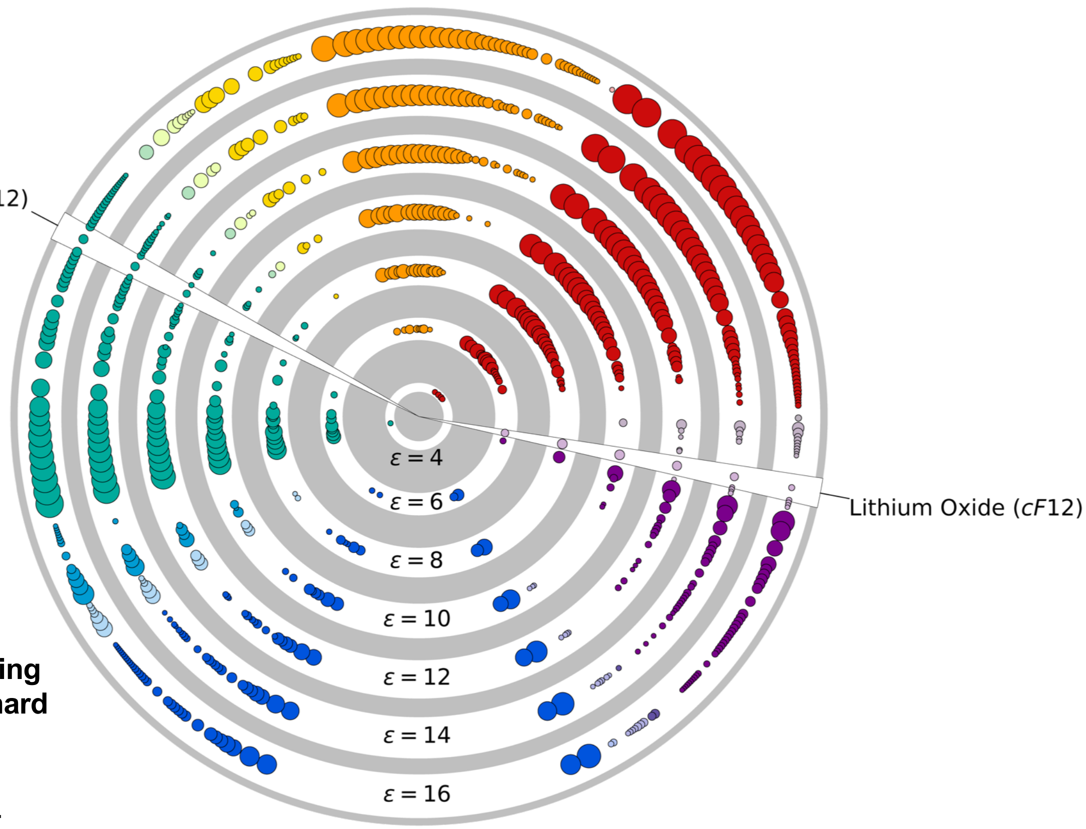
Results

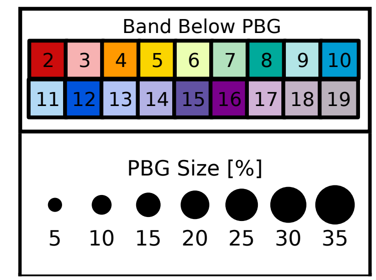




c-OT_2

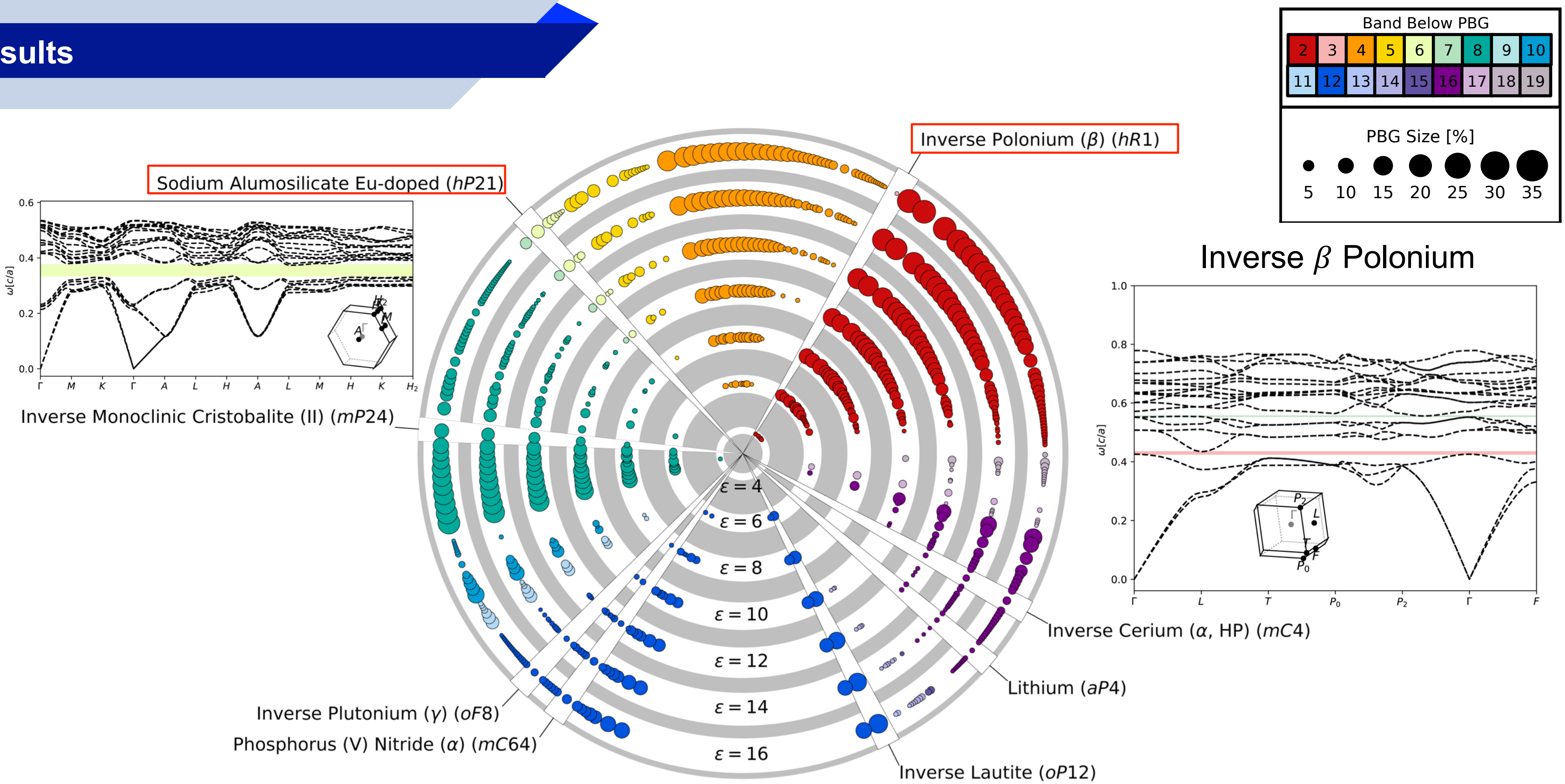
Self-assembly of a space-tessellating structure in the binary system of hard tetrahedra and octahedra.
Cadotte, Andrew T., et al.
Soft matter 12.34 (2016): 7073-7078.





The diversity of three-dimensional photonic crystals
RKC, et al. *Nature Communications* 12, https://doi.org/10. 1038/s41467-021-22809-6 (2021).

Results



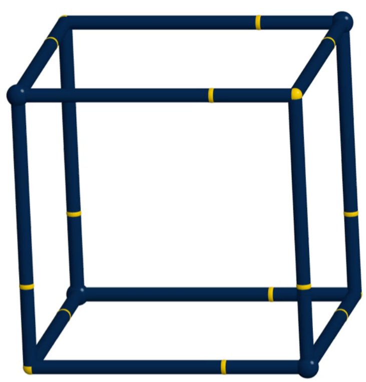
The diversity of three-dimensional photonic crystals
RKC, et al. *Nature Communications* 12, https://doi.org/10. 1038/s41467-021-22809-6 (2021).

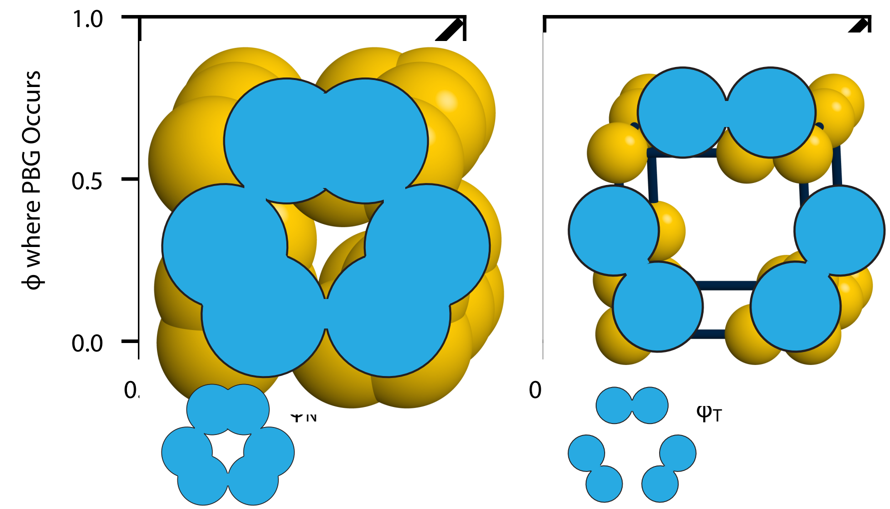
Are previous design rules predictive of this set of photonic crystals?

Results

Photonic band gaps can occur when the high dielectric regions are either connected or disconnected and a full network is not required.

Photonic band gaps are best supported in lattices where high dielectric regions are continuously connected.





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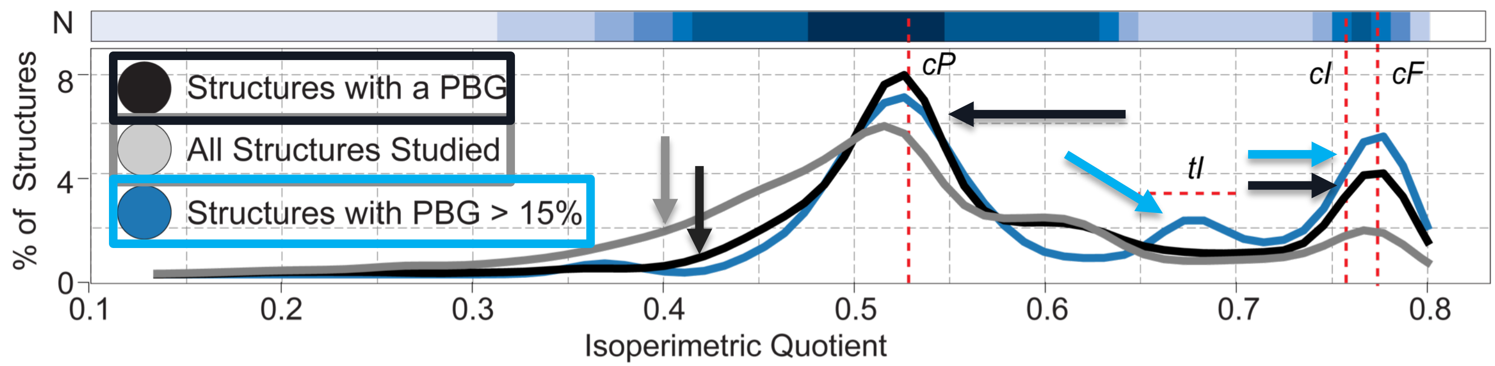
RKC, et al. *Nature Communications* 12, https://doi.org/10. 1038/s41467-021-22809-6 (2021).

PBG are more likely to be found in *high symmetry* lattices, but can be found in highly asymmetric lattices.

PBG are most easily supported in lattices with more spherical Brillouin zones.

Sphericity of the Brillouin Zone



	aP	*mP*	*mC*	*oP*	*oC*	*oF*	*oI*	*oA*	*tP*	*tI*	*hP*	*hR*	*cP*	*cF*	*cI*
# Structures	60	156	192	356	164	86	104	36	390	246	404	130	184	114	90
# with PBG	2	11	9	24	10	7	5	4	39	41	58	33	58	47	19
% with PBG	3%	7%	5%	7%	6%	8%	5%	11%	10%	17%	14%	25%	32%	41%	21%

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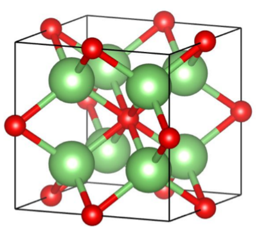
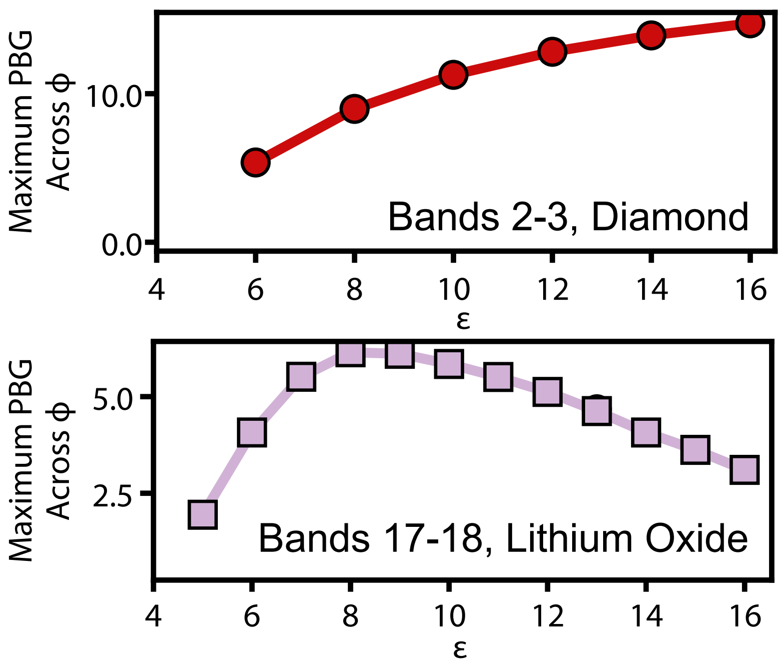
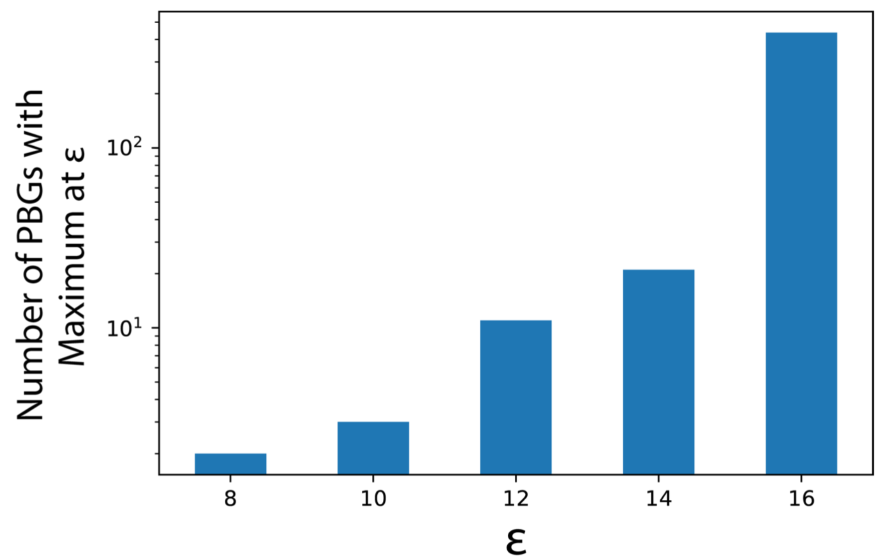
RKC, et al. *Nature Communications* 12, https://doi.org/10. 1038/s41467-021-22809-6 (2021).

Results

Higher dielectric constant generally leads to a larger gap, but not always.





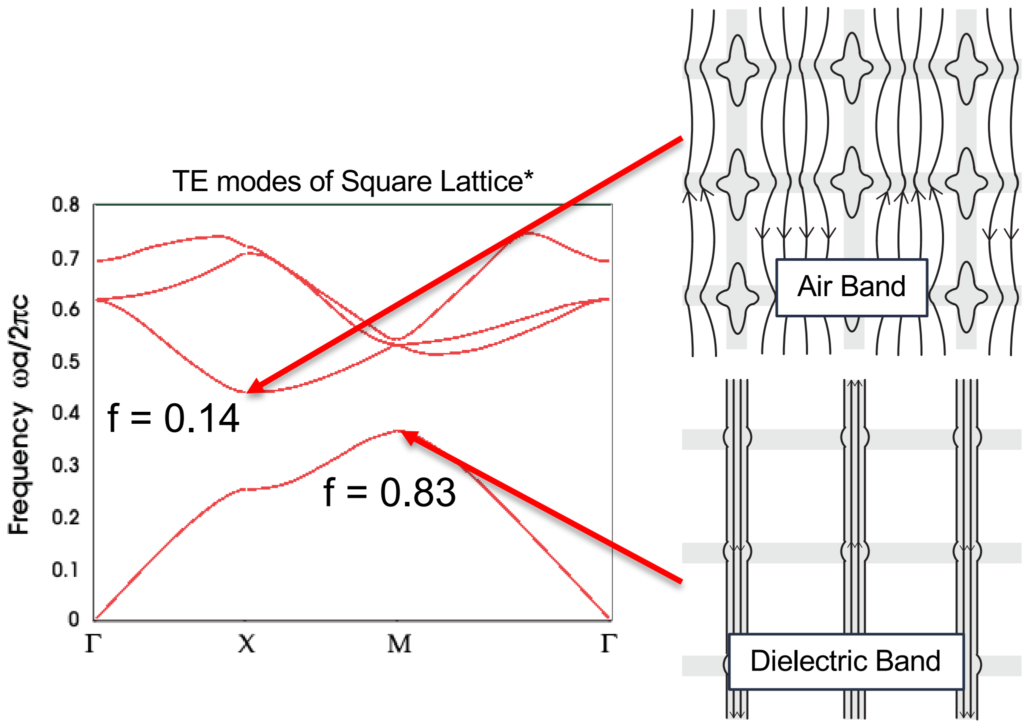


For more detailed analysis, see SI Fig. 9 of Cersonsky, et al., 2021.

Why?

Because 2D is not the same as 3D.

Field Analysis of Photonic Crystals



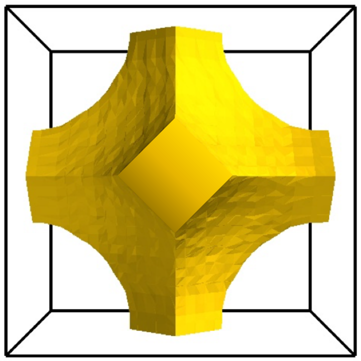
$$f = \frac{\int_{V_\varepsilon} \mathbf{E}^*(\mathbf{r}) \cdot \mathbf{D}(\mathbf{r}) d\mathbf{r}}{\int \mathbf{E}^*(\mathbf{r}) \cdot \mathbf{D}(\mathbf{r}) d\mathbf{r}}$$

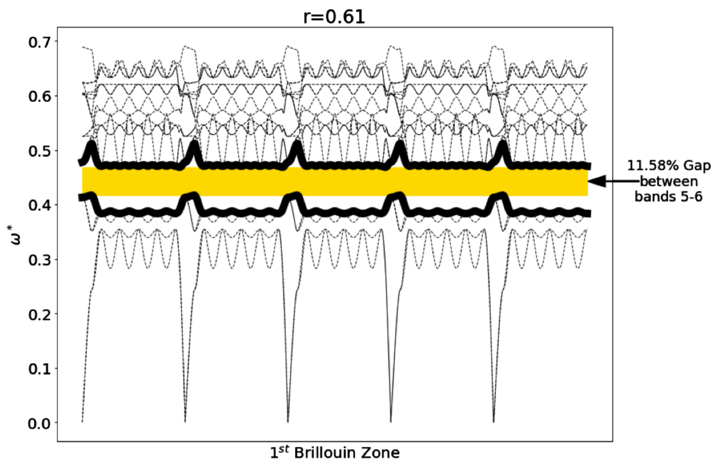
f	"concentration factor", fraction of electric energy found in the high dielectric material
V_ε	region with the higher dielectric constant
$\mathbf{E}^*(\mathbf{r})$	conjugate of the time-independent electric field
$\mathbf{D}(\mathbf{r})$	time-independent displacement field

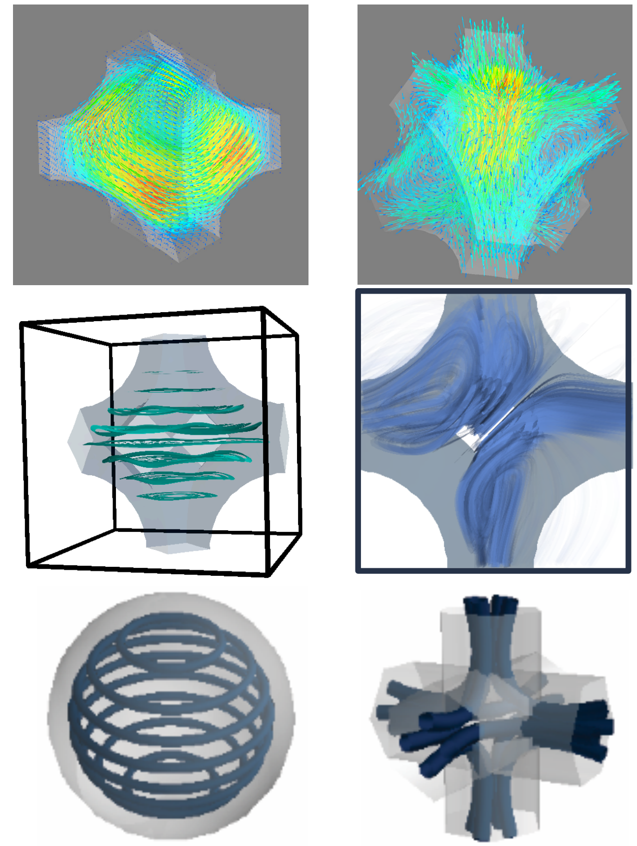
Nature of the photonic band gap: some insights from a field analysis
R. D. Meade, A. M. Rappe, K. D. Brommer, and J. D. Joannopoulos
Journal of the Optical Society of America B (1993) 10 (2), pp. 328-332

*One can conduct similar analysis for the transverse magnetic (TM) polarization.

Field Analysis of Photonic Crystals







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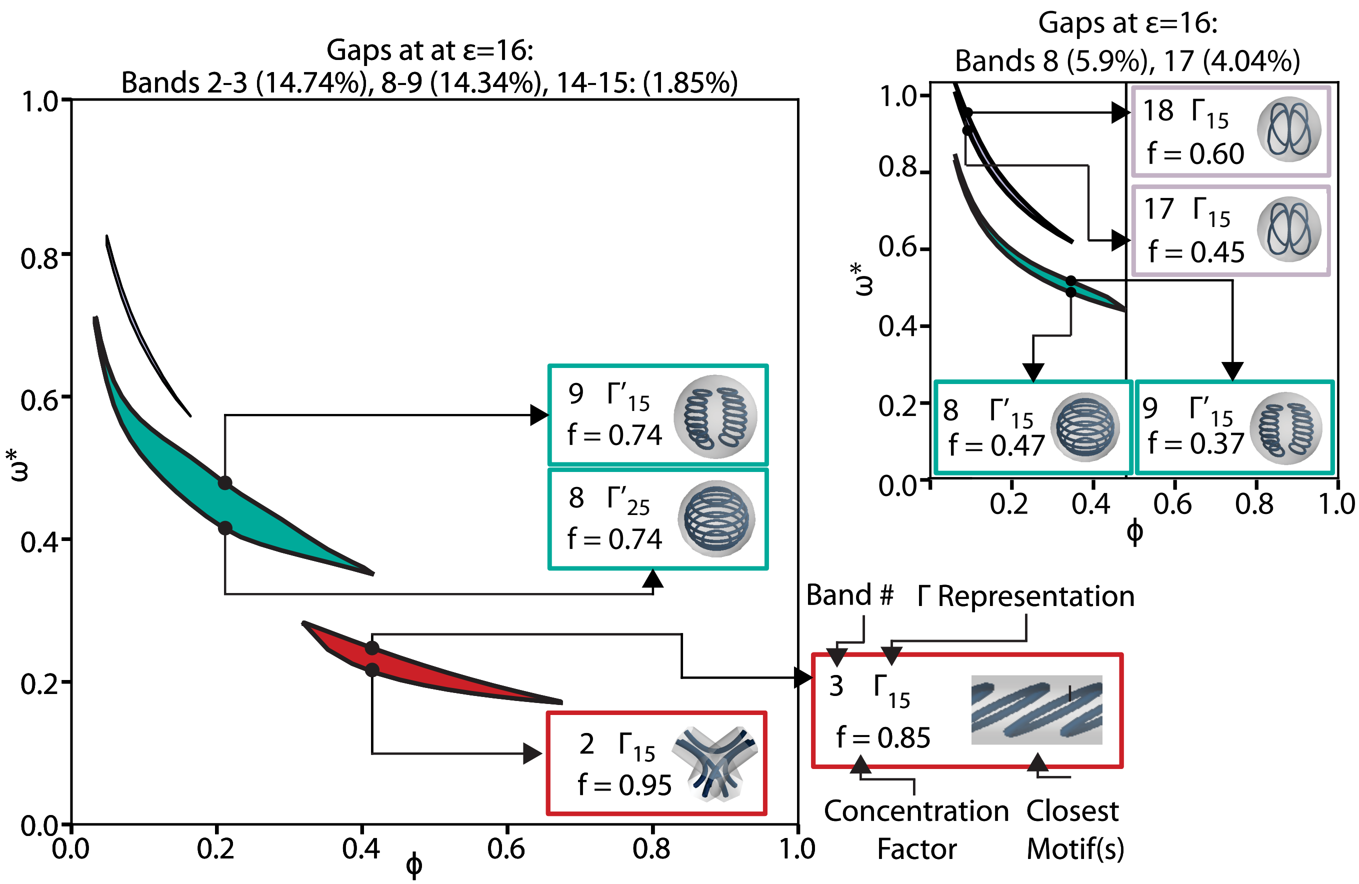
Field Analysis of Photonic Crystals



The diversity of three-dimensional photonic crystals
RKC, et al. *Nature Communications* 12, https://doi.org/10. 1038/s41467-021-22809-6 (2021).

We have learned a lot about how to design 3D photonic crystals from the 2D analogs, yet many rules are “bent” in 3D.

The space of photonic crystals available is diverse, with many that we already know how to make on colloidal length scale.

Designing Nanoparticles for Self-Assembly of Novel (Photonic) Materials

My website for more info and slides from today's talk

The diversity of three-dimensional photonic crystals
RK Cersonsky, J Antonaglia, BD Dice, SC 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

Designing Nanoparticles for Self-Assembly of Novel (Photonic) Materials

- **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."

Engaging the Community in STEM Outreach

- AT Travitz, AJ Muniz, JK Beckwith, **RK Cersonsky.** *ASEE.* doi:10.18260/1-2--35030 (2020).
- **RK Cersonsky**, LL Foster, T Ahn, RJ Hall, HL Van Der Laan, TF Scott. *J. of Chem. Ed.* **94,** 1639–1646 (2017).

Machine Learning for Structure-Property Relationships

- **RK Cersonsky,** BA Helfrecht, EA Engel, S Kliavinek, M Ceriotti. *Machine Learning: Science and Technology.* doi:10.1088/2632- 2153/abfe7c (2021).
- BA Helfrecht, **RK Cersonsky,** G Fraux, M Ceriotti, *Machine Learning: Science and Technology* **1,** 045021 (2020).
- G Fraux, **RK Cersonsky,** M Ceriotti, Chemiscope: *JOSS,* **5,** 2117 (2020).

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