Design of Super Functional Materials and Devices using Artificial Intelligence

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KIAS, June 26–30, 2023

Contents

- Background {artificial intelligence}
- Evolutionary learning
- Artificial neural networks
- Applications
- [RDFSEARCH, AMADEUS]

What's next?

As DeepMind co-founder, Demis Hassabis explains, Zero was not programmed to understand Go specifically, it could be reprogrammed to discover information in other fields: drug discovery, protein folding, quantum chemistry, particle physics, and material design.

2011: Relu
2012: CNN, Alex Net
2013: VAE
2014: GAN
2015: TF
2016: alpha Go
2017: Zero, cycleGAN
2018: alpha fold
2020: alpha fold 2
2021: Ramanujan,
Floor planning,
Nowcasting,
DM21
2022: alpha tensor
ChatGPT

Breakthrough Prize

Demis Hassabis

https://becominghuman.ai/what-does-deepminds-latest-publication-mean-for-a-i-d496ab06d61f

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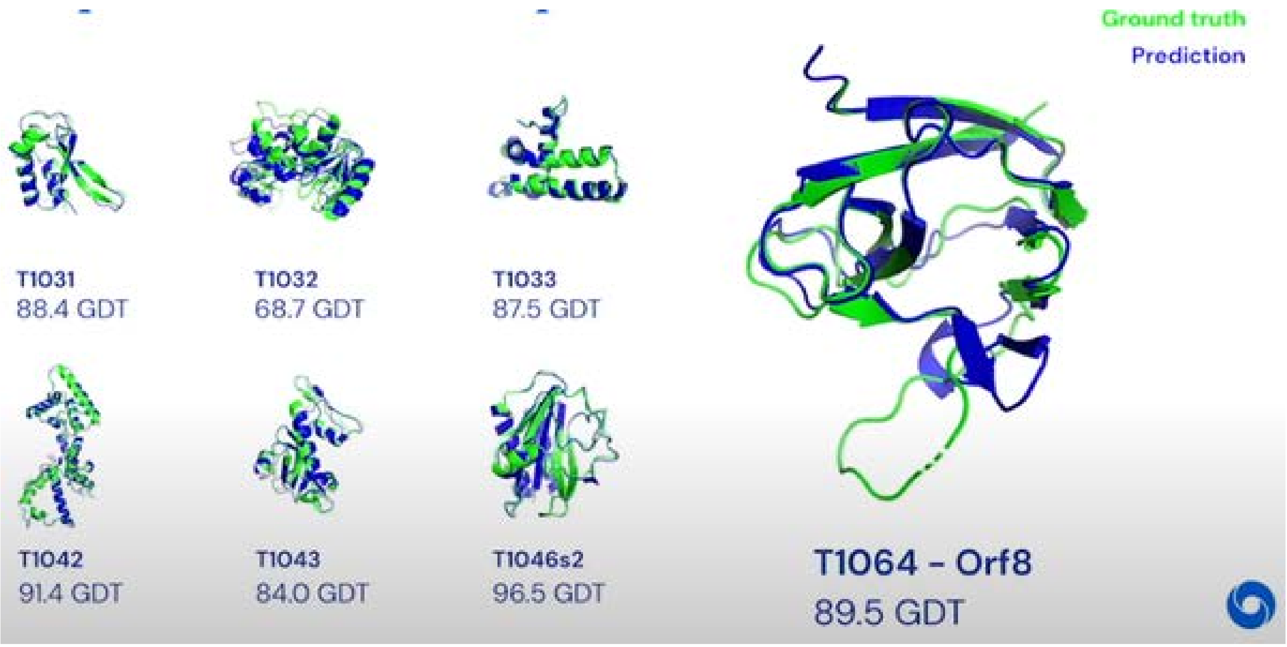
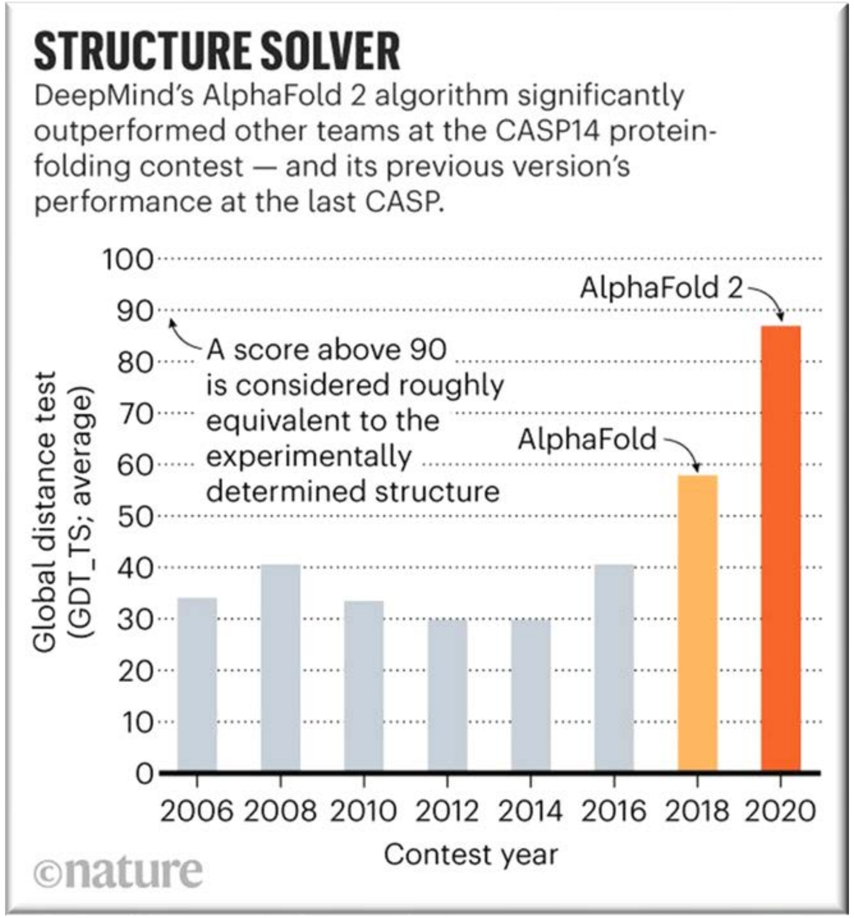
Protein folding problem





RoseTTAFold
ESMFold, Meta's Rival To AlphaFold

Isomorphic Labs, 갤럭스, 굳인텔리젼스, 힛츠, 아론티어, 스탠다임

Nature **596**, 583 (2021). Science **373**, 871 (2021).

Nature **596**, 583 (2021). Science **373**, 871 (2021).

얼마나 창의적인가? 새로운 수학공식들

$$\pi = \sum_{n=0}^{\infty} \frac{1}{16^n} \left(\frac{4}{8n+1} - \frac{2}{8n+4} - \frac{1}{8n+5} - \frac{1}{8n+6} \right).$$

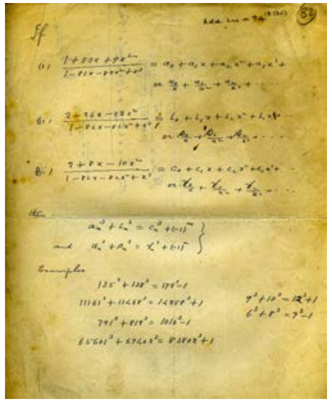
$$\frac{8}{\pi^2} = 1 - \cfrac{2\times 1^4 - 1^3}{7 - \cfrac{2\times 2^4 - 2^3}{19 - \cfrac{2\times 3^4 - 3^3}{37 - \cfrac{2\times 4^4 - 4^3}{\cdots}}}}$$

$$\frac{12}{7\zeta(3)} = 1\times 2 - \cfrac{16\times 1^6}{3\times 12 - \cfrac{16\times 2^6}{5\times 32 - \cfrac{16\times 3^6}{7\times 62 - \cfrac{16\times 4^6}{\cdots}}}}$$

$$\frac{8}{7\zeta(3)} = 1\times 1 - \cfrac{1^6}{3\times 7 - \cfrac{2^6}{5\times 19 - \cfrac{3^6}{7\times 37 - \cfrac{4^6}{\cdots}}}}$$

$$\frac{2}{-1+2G} = 3 + 0\times 7 - \cfrac{6\times 1^3}{3 + 1\times 10 - \cfrac{8\times 2^3}{3 + 2\times 13 - \cfrac{10\times 3^3}{\cdots}}} \qquad (4)$$

Srinivasa Ramanujan: The mathematical genius who credited his 3900 formulae to visions from Goddess Mahalakshmi.



Nature **590**, 67 (2021).

Floor planning

Nature **594**, 207 (2021).

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Generative models for nowcasting

2012년이 딥러닝의 원년이다.
2011년 **Relu** 함수의 출현 **: vanishing gradient problem** 해결, 표현력이 높은 딥러닝이 시작됨.
2012년 **Dropout** 방법의 출현 **: overfitting problem** 해결, 정규화된 훈련이 가능함.
2012년 **CNN** 출현 : 방대한 이미지 데이터 처리 문제 해결, 비대칭 데이터에 대한 처리가 가능함.
2013년 **VAE** 출현: 생성모델로서 다양한 가능성을 제안함.
2014년 **GAN** 출현: 생성모델로서 많은 응용 가능성을 제안함.
2015년 **TensorFlow** 구현의 출현과 보급 : 실질적인 딥러닝의 민주화가 단행됨.
2016년 알파고 출현 : 바둑 정복
2017년 알파고 제로 출현 **: tabula rasa, first-principles** 방법을 이용하여 바둑 정복, 진정한 바둑의 정복이 가능함. 기보없이 바둑 정복함. 프로기사에게 절대로 지지 않는 사실상 바둑의 신이 탄생함. 바둑의 역사 5000년 Mastering the game of Go without human knowledge | Nature http://incredible.egloos.com/7372719
2017년 cycleGAN 출현 http://incredible.egloos.com/7530913
2018년 알파폴드 출현
2020년 알파폴드 2 출현 http://incredible.egloos.com/7479504 Highly accurate protein structure prediction with AlphaFold | Nature
2021년 라마누잔 기계 (수학공식 생성기) http://incredible.egloos.com/7511552 Generating conjectures on fundamental constants with the Ramanujan Machine | Nature
2021년 플로어플랜닝 (반도체 칩 설계) A graph placement methodology for fast chip design | Nature
2021년 나우캐스팅 (단기 일기예보) https://www.nature.com/articles/s41586-021-03854-z
2022년 알파텐서, ChatGPT

Nature **597**, 672 (2021).

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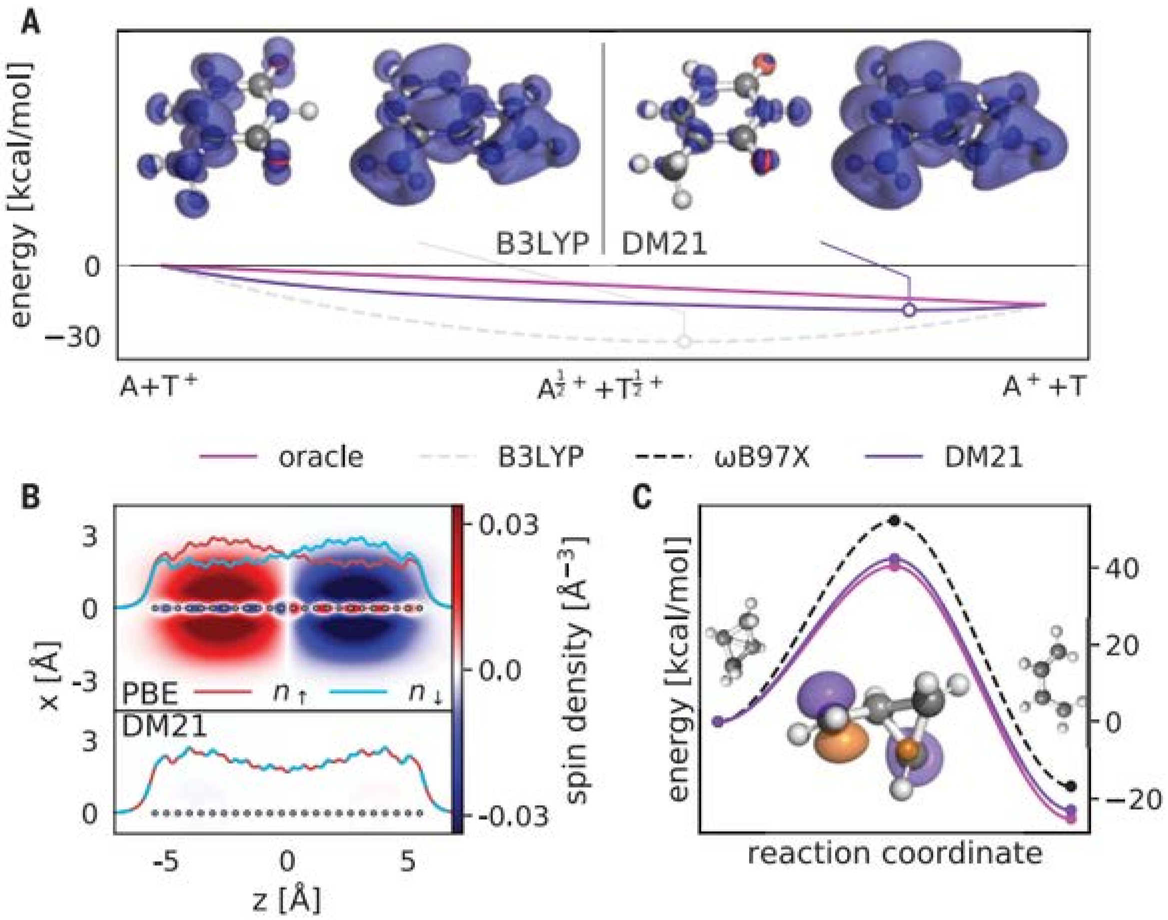
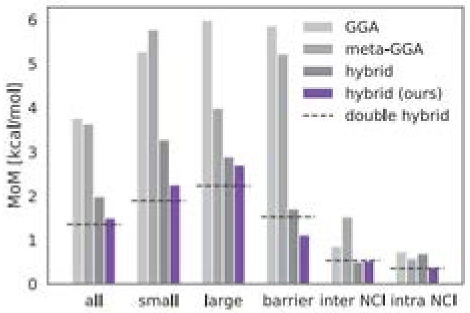
Density functionals



A

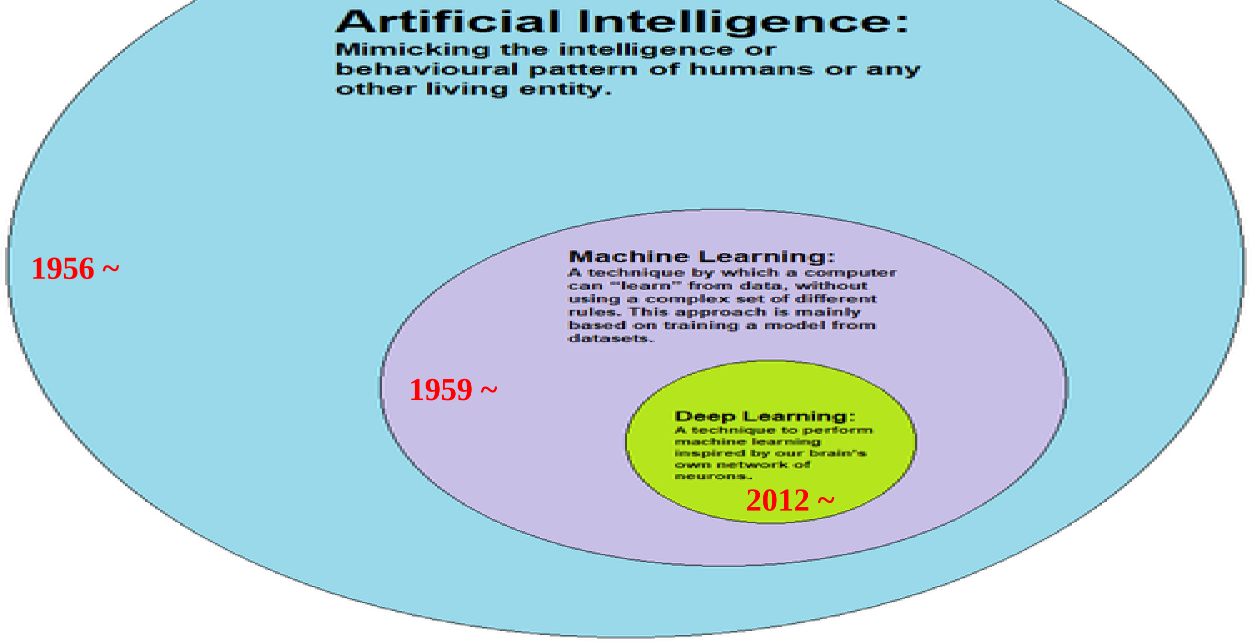


B

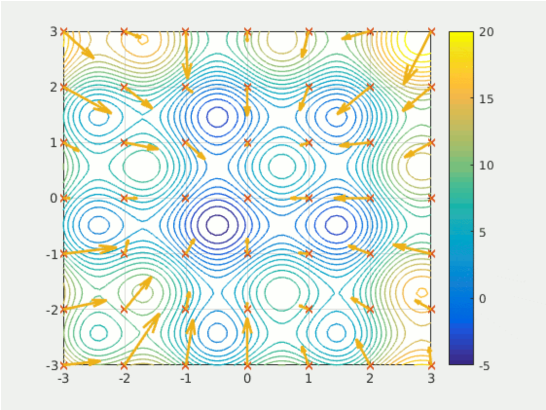
	GMTKN55 MoM	BBB	QM9
SCAN(:D3$_{BJ}$)	3.63	52.90	3.57
ωB97X(-V)	2.45	70.28	2.13
M06-2X	2.08	64.50	2.20
PW6B95:D3$_0$	1.98	57.81	2.24
DM21	**1.50**	**13.20**	**1.66**

Science **374**, 1385 (2021).

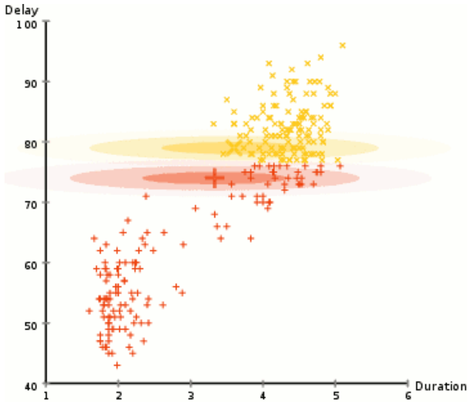
AI tools



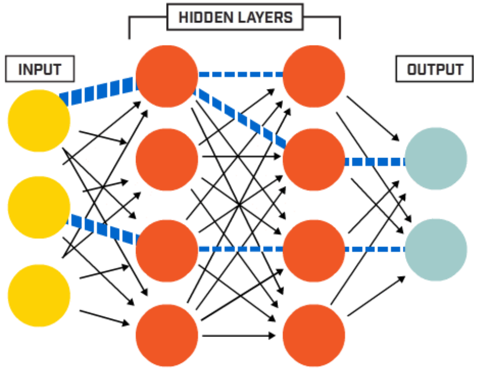
Search and optimization



Classifiers and statistical learning methods



Artificial neural networks



The overall research goal of artificial intelligence is to create technology that allows computers and machines to function in an intelligent manner.

https://en.wikipedia.org/wiki/Artificial_intelligence

Forms of Machine Learning

1. Supervised learning

Four learning types

2. Unsupervised learning

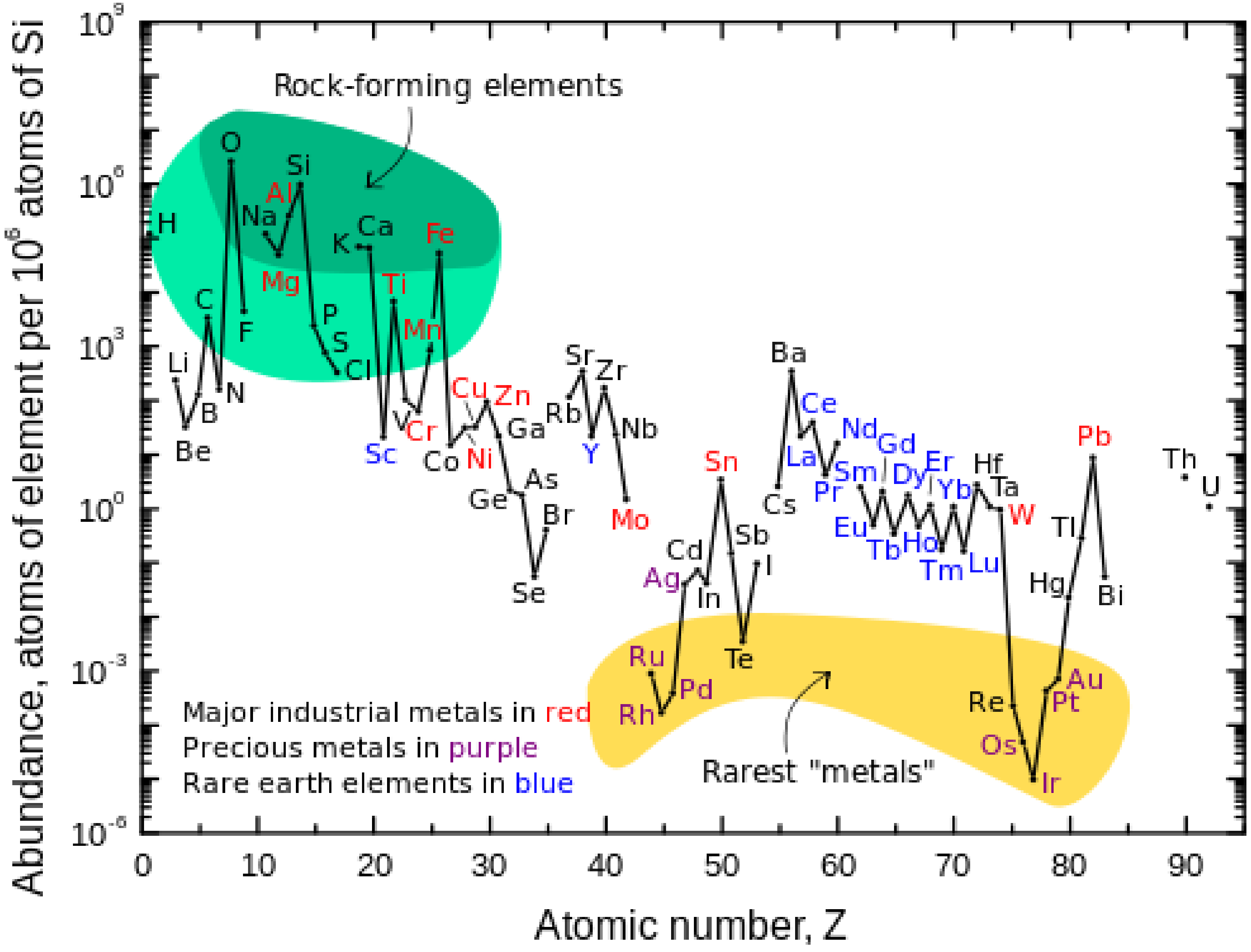
3. Reinforcement learning

4. Evolutionary learning

Three elements

Learning task = {1. Representation} $\oplus$ {2. Evaluation} $\oplus$ {3. Optimization}

Abundance, crust, …



http://en.wikipedia.org/wiki/Crust_(geology)

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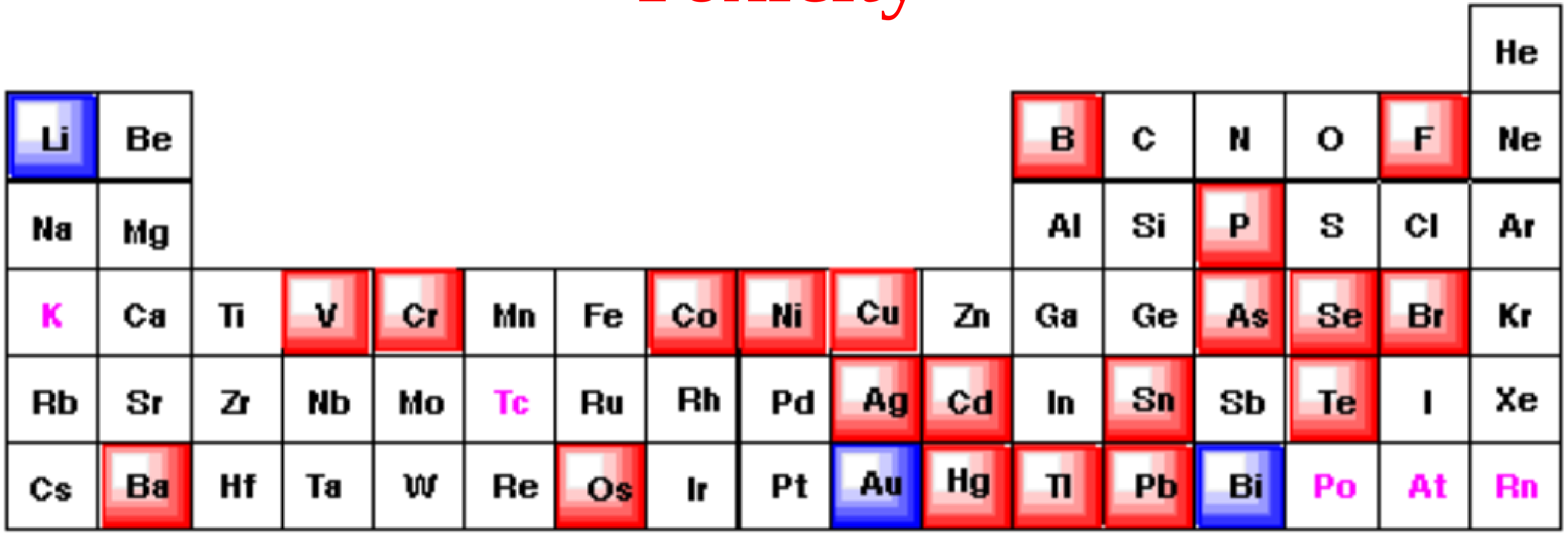
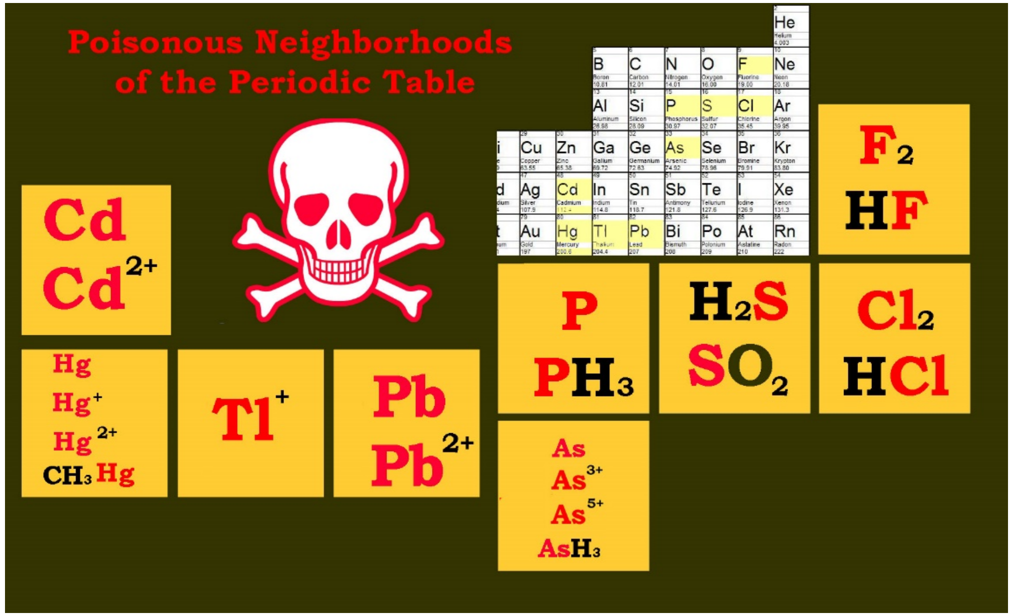
Toxicity



He
Li Be B C N O F Ne
Na Mg Al Si P S Cl Ar
K Ca Ti V Cr Mn Fe Co Ni Cu Zn Ga Ge As Se Br Kr
Rb Sr Zr Nb Mo Tc Ru Rh Pd Ag Cd In Sn Sb Te I Xe
Cs Ba Hf Ta W Re Os Ir Pt Au Hg Tl Pb Bi Po At Rn



Poisonous Neighborhoods
of the Periodic Table
Cd
Cd^{2+}
Hg
Hg^{+}
Hg^{2+}
CH_3Hg
Tl^{+}
Pb
Pb^{2+}
P
PH_3
H_2S
SO_2
F_2
HF
Cl_2
HCl
As
As^{3+}
As^{5+}
AsH_3

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Approaches

- Known materials → High-throughput calculations [first-principles]
- Known materials → encoding → regression/classification models → prediction for existing and/or known materials → first-principles calculations : Materials repurposing/repositioning [artificial neural networks]
- Unknown materials → Generative models[exploration][database]
- Unknown materials → Design via global optimization[design][tabula rasa, first-principles]

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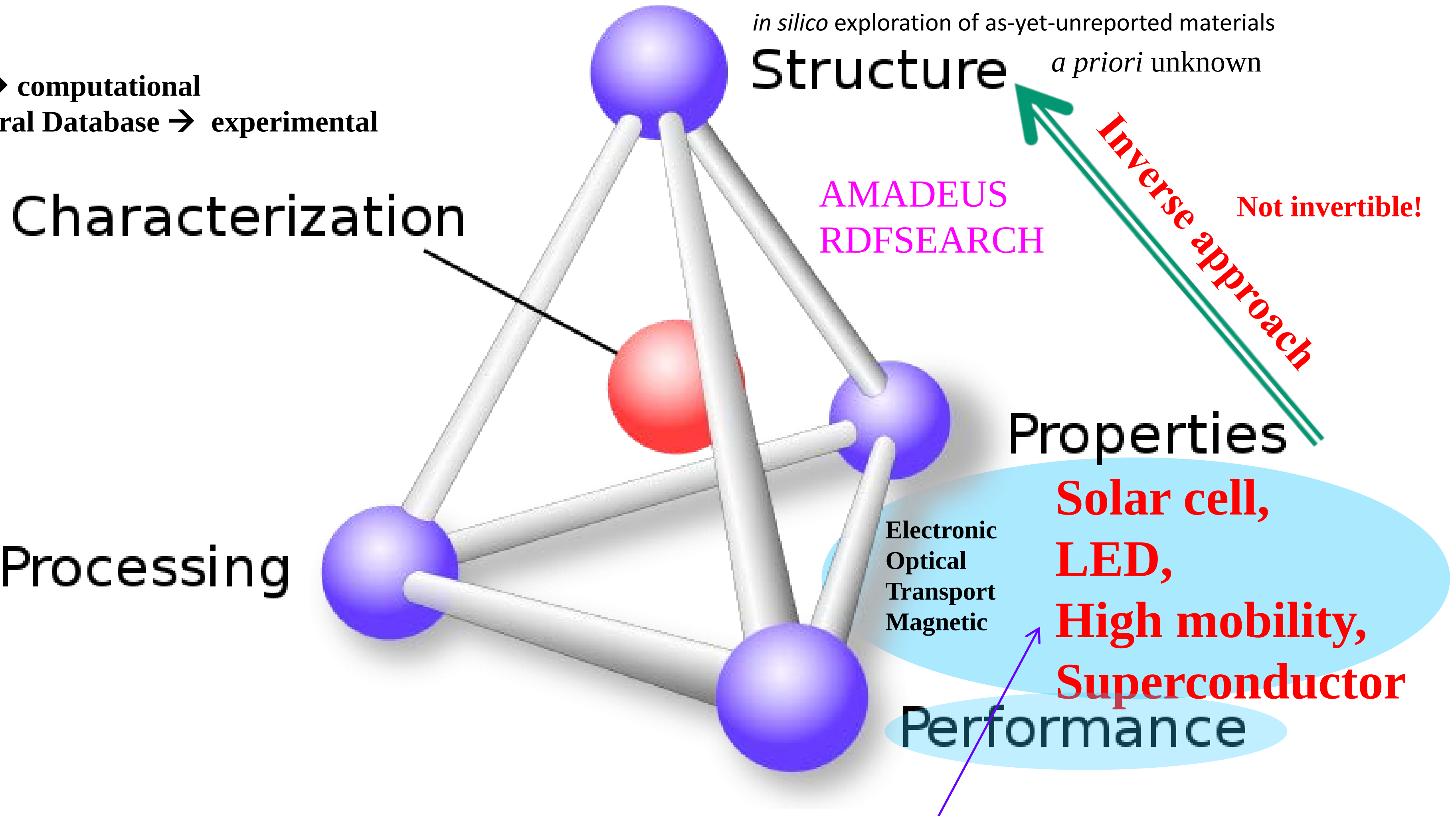
The understanding of processing-structure-properties relationships is called the materials paradigm.

in silico exploration of as-yet-unreported materials

Materials Project → computational
Cambridge Structural Database → experimental



VESTA
VASP
Quantum Espresso
Mechanical stability
Phonopy
Wannier90
EPW
WannierTools
BerkeleyGW
BoltzTrap
PyProcar

Nature **402**, 60 (1999), Nature Rev. Chem. **2**, 0121 (2018).
https://en.wikipedia.org/wiki/Materials_science

Topological materials, Chern insulator?

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Conformational Space Annealing (CSA)

- Based on genetic algorithm(GA) → maintain a pool of conformations (bank) and new conformations are obtained by mating (crossover) and mutation (small perturbation)
- Consider only conformational space of local minima (as in MCM)
- Diversity of the bank is directly controlled by introducing the concept of *distance* between the conformations
- Narrows the search to smaller region while maintaining diversity of sampling
- Key idea : GA + annealing in conformational space

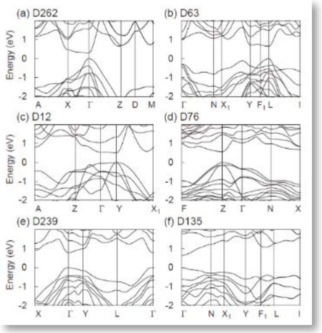
Protein structure prediction (modeling) {CASP experiments}
X-ray data → crystal structure determination
NMR → molecule structure determination
Bioinformatics
LJ clusters
Travelling salesman problem
***Ab initio* materials design (super functional materials)**
Pathway sampling (Action-CSA)
……..

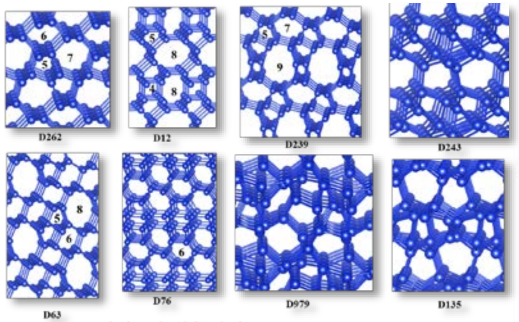
Comput. Phys. Commun. **203**, 110 (2016).
Phys. Rev. Lett. **91**, 080201 (2003).
J. Comput. Chem. **18**, 1222 (1997).

Ab initio materials design using conformational space annealing (AMADEUS)

$$\text{Atomic configuration} \longrightarrow \text{Electronic structure} \qquad (1)$$

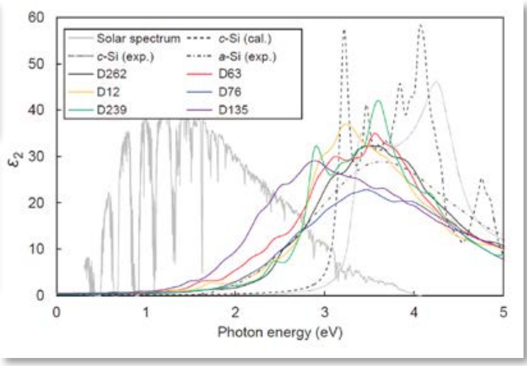
$$\text{Electronic structure} \longrightarrow \text{Atomic configuration} \qquad (2)$$

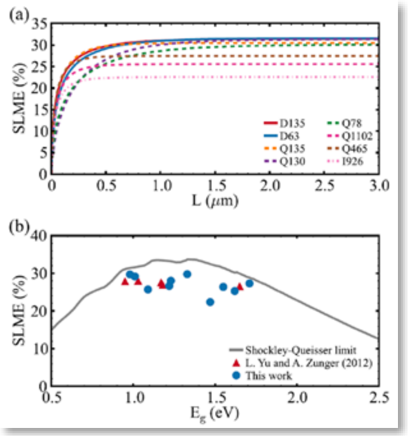




- 8 crystals with direct band gaps
- 20 crystals with quasi-direct band gaps
- No coordination defect in all the designed structures

Comput. Phys. Commun., *in press* (2016).





DFT ⟷ Conformational Space Annealing ⟷ Crystal structures → *GW*-BSE ⟷ SLME

Crystal structures → Lattice dynamics, Molecular dynamics

https://github.com/inholeegithub/winter2022

Comput. Phys. Commun. **203**, 110 (2016).

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Applications

- Solar cell (Si): Phys. Rev. B **90**, 115209 (2014), Sci. Rep. **5**, 18086 (2015), Comp. Phys. Commun. **203**, 110 (2016).
- LED (C): Phys. Rev. B **93**, 085201 (2016).
- High-mobility [green phosphorus] (P): J. Phys. Chem. Lett. **8**, 4627 (2017).
- Topological materials (Si, C, $Ag_2Se_{0.5}Te_{0.5}$): J. Phys. Chem. C **123**, 1839 (2019), NPG Asia Materials **9**, e361 (2017), Nanoscale **11**, 5171 (2019).
- Structure searches (B): Sci. Rep. **7**, 7279 (2017), NPG Asia Materials **9**, e400 (2017), arXiv:1902.08390
- Superconductivity (Si): Phys. Rev. Lett. **120**, 157001 (2018).
- Topological superconductivity (Si): Phys. Rev. Mat. **5**, 104802 (2021); Phys. Rev. B **107**, 115127 (2023).

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ThisPersonDoesNotExist.com uses AI to generate endless fake faces

This X does not exist

Materials Project → computational
Cambridge Structural Database → experimental

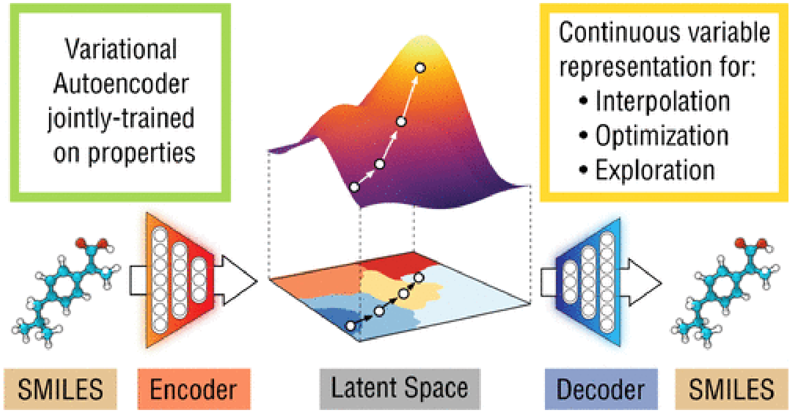
[This X Does Not Exist](#)
[Artificial Intelligence Songwriter – These Lyrics Do Not Exist](#)
[This Chemical Does Not Exist](#)
[thisartworkdoesnotexist.com (512×512)](#)
[This Person Does Not Exist](#)
[This Music Video Does Not Exist](#)

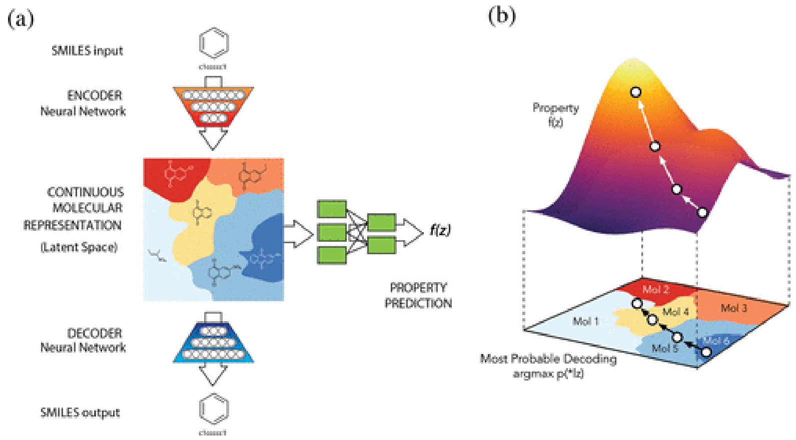
Neural Style Transfer
Gram matrix

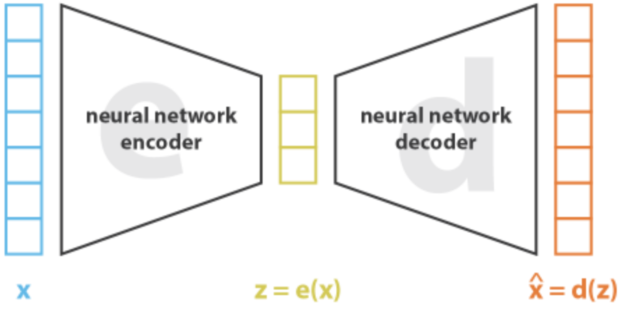
Boltzmann machine, GAN, VAE, RNN, PixelCNN

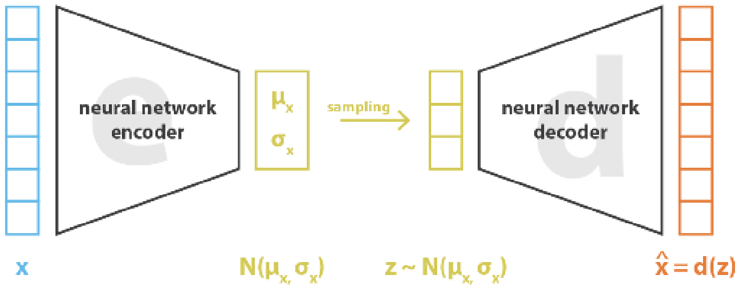
Generative models

Automatic Chemical Design Using a Data-Driven Continuous Representation of Molecules







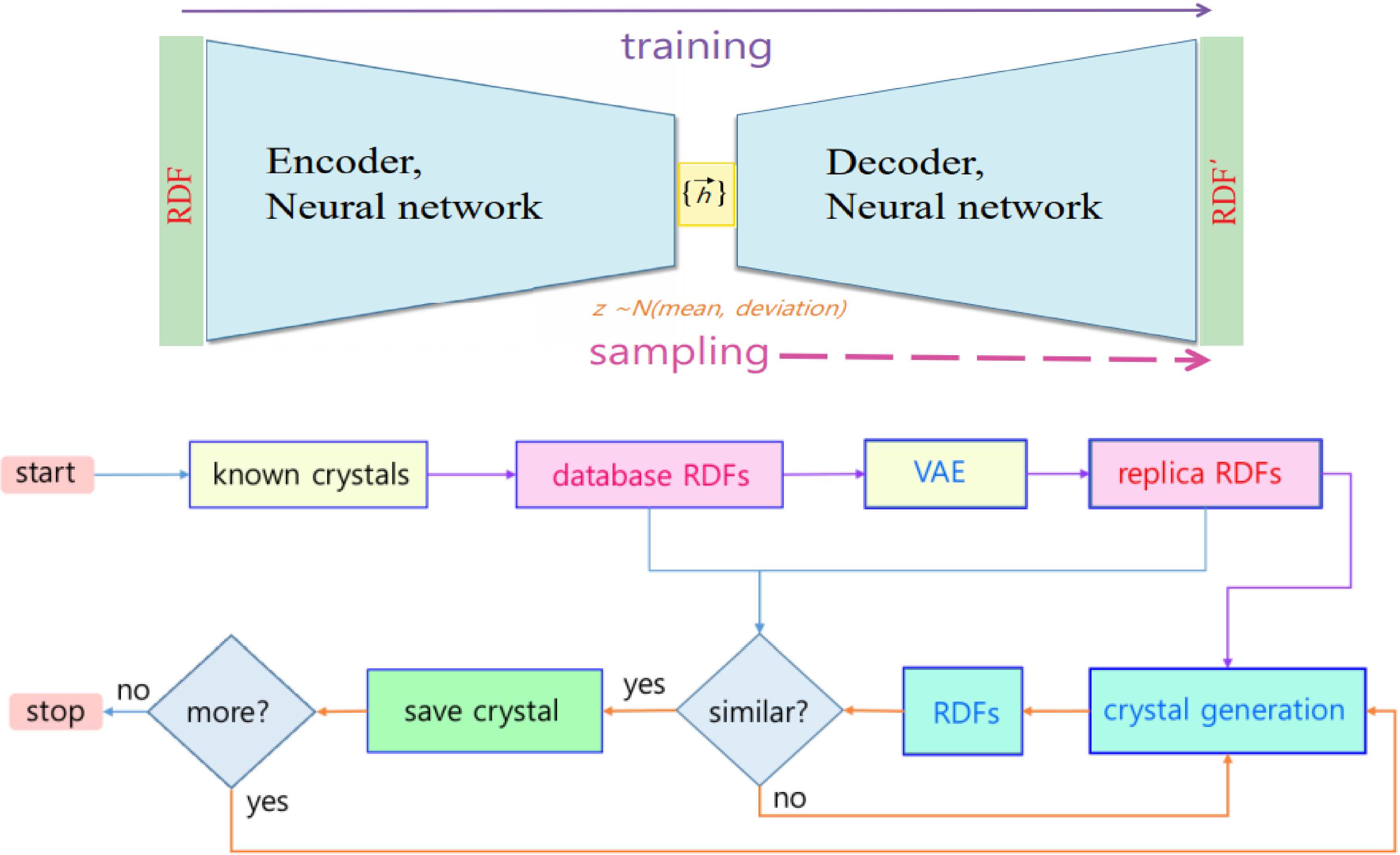


$$\text{loss} = \| x - \hat{x} \|^2 = \| x - d(z) \|^2 = \| x - d(e(x)) \|^2$$

$$\text{loss} = \| x - \hat{x} \|^2 + KL[\,N(\mu_x, \sigma_x), N(0, I)\,] = \| x - d(z) \|^2 + KL[\,N(\mu_x, \sigma_x), N(0, I)\,]$$

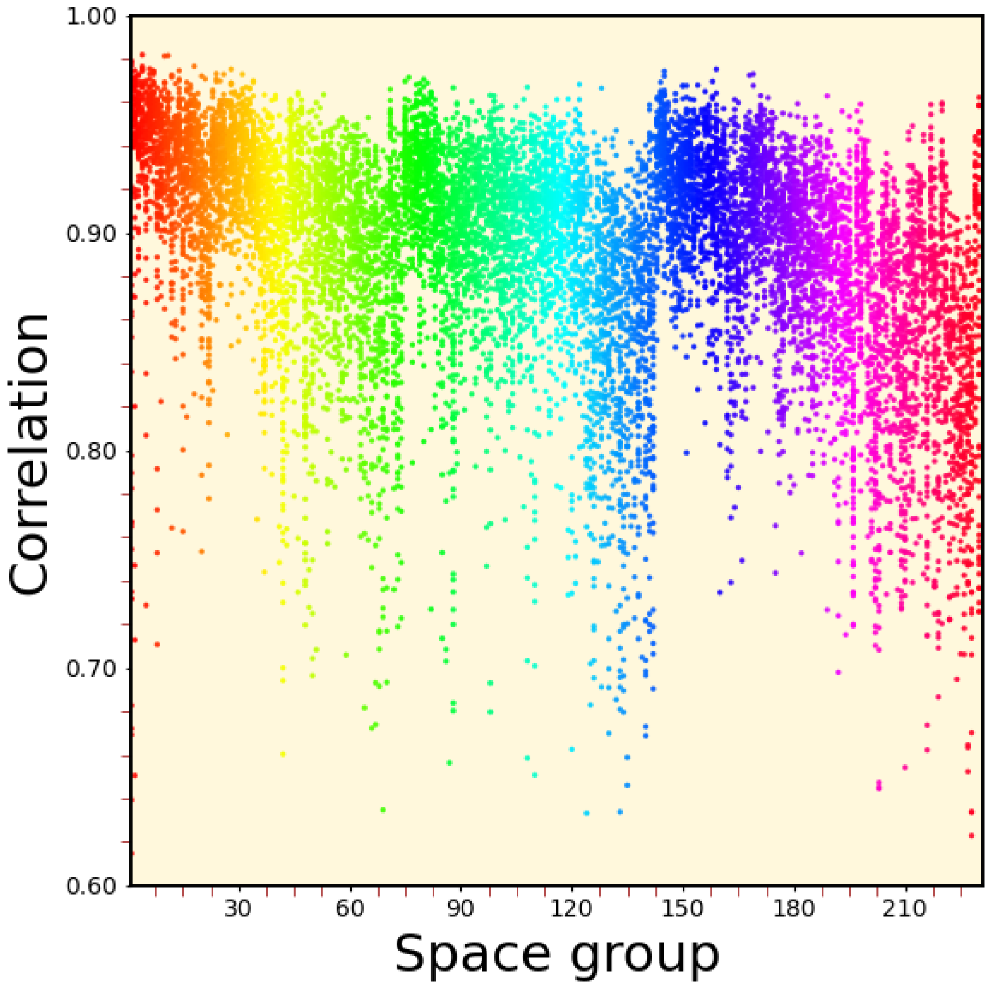
https://towardsdatascience.com/understanding-variational-autoencoders-vaes-f70510919f73
ACS Cent. Sci. **4**, 268 (2018).

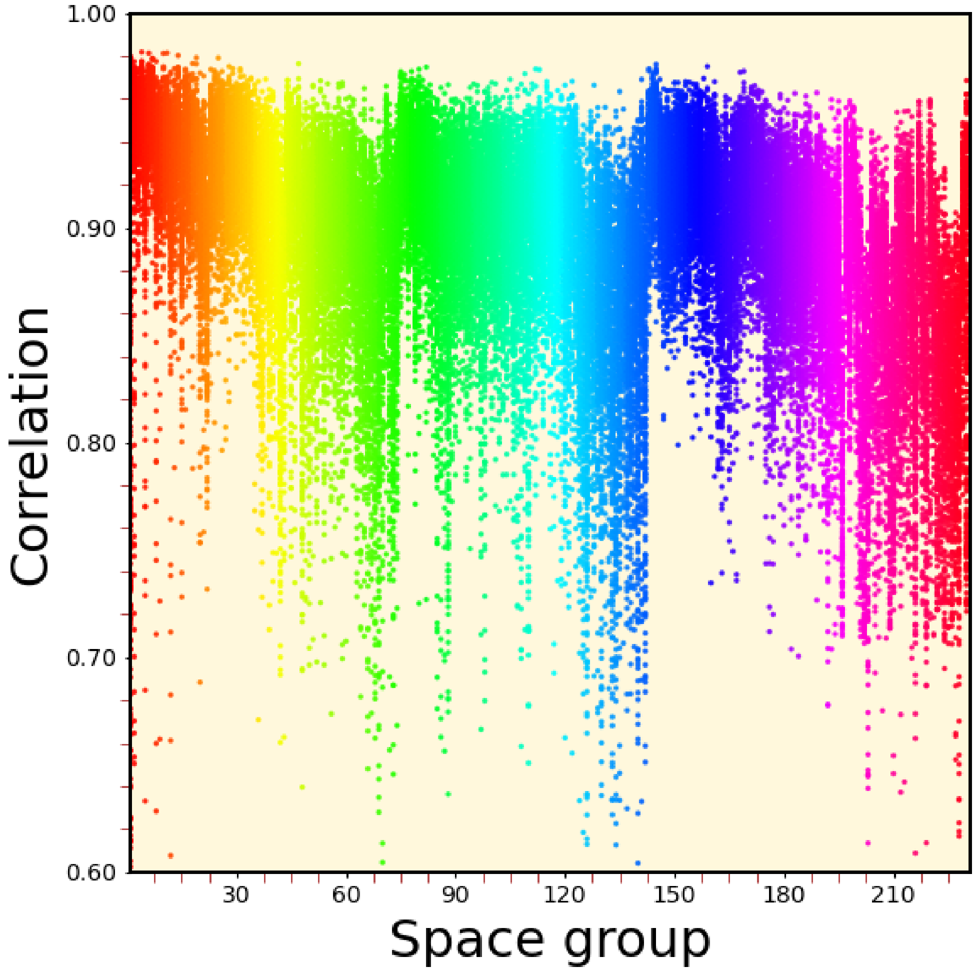
Crystal structure prediction in a continuous representation space



https://github.com/inholeegithub/winter2022
Comput. Mat. Sci. **194**, 110436 (2021).

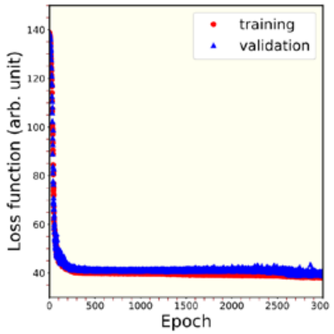
Crystal structure prediction in a continuous representation space

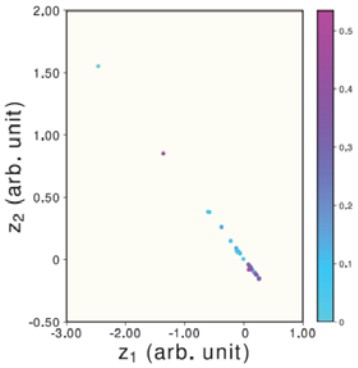


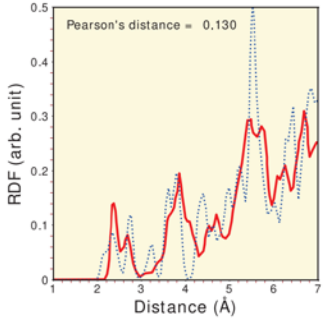


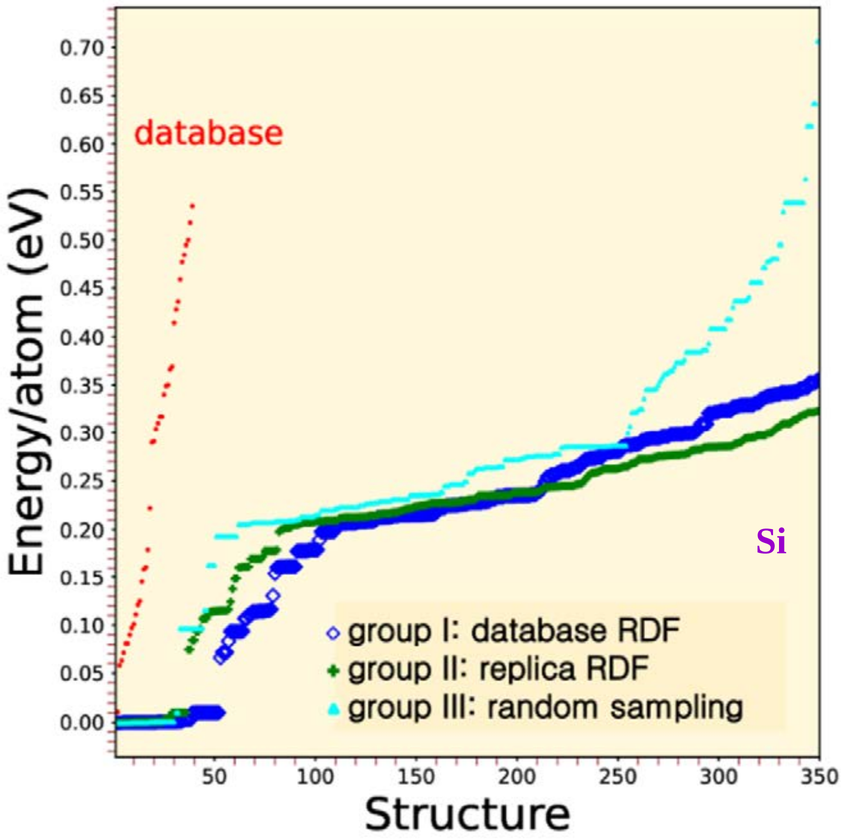
https://github.com/inholeegithub/winter2022
Comput. Mat. Sci. **194**, 110436 (2021).

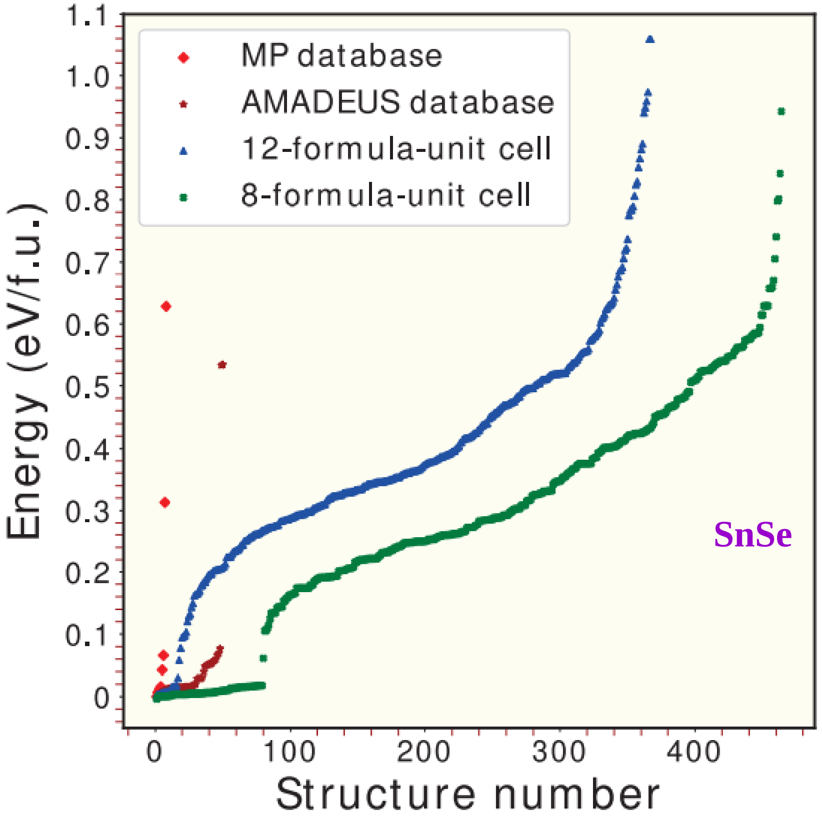
Data-driven continuous representation







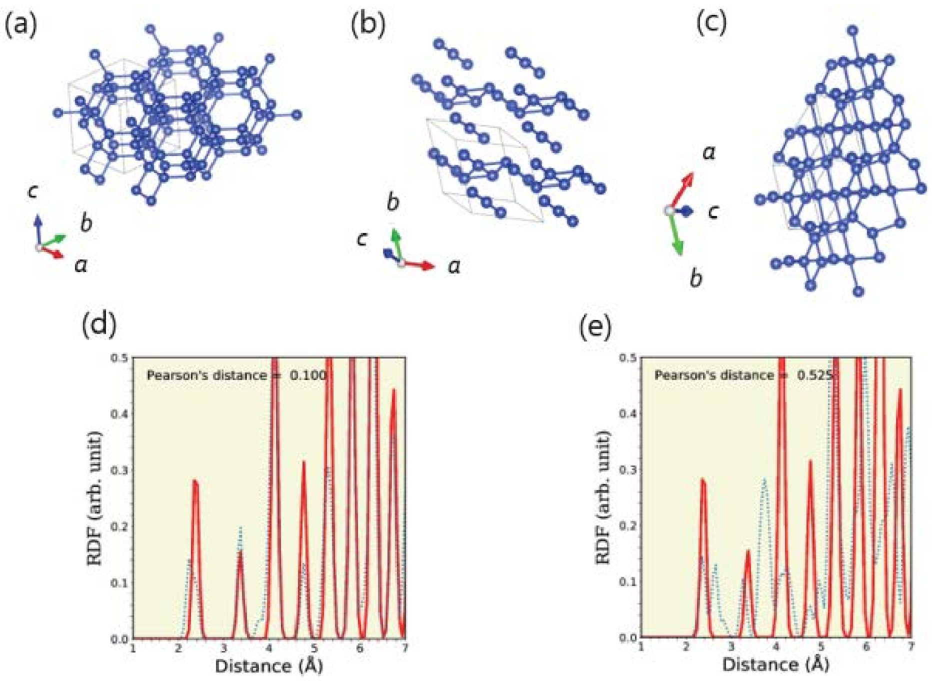


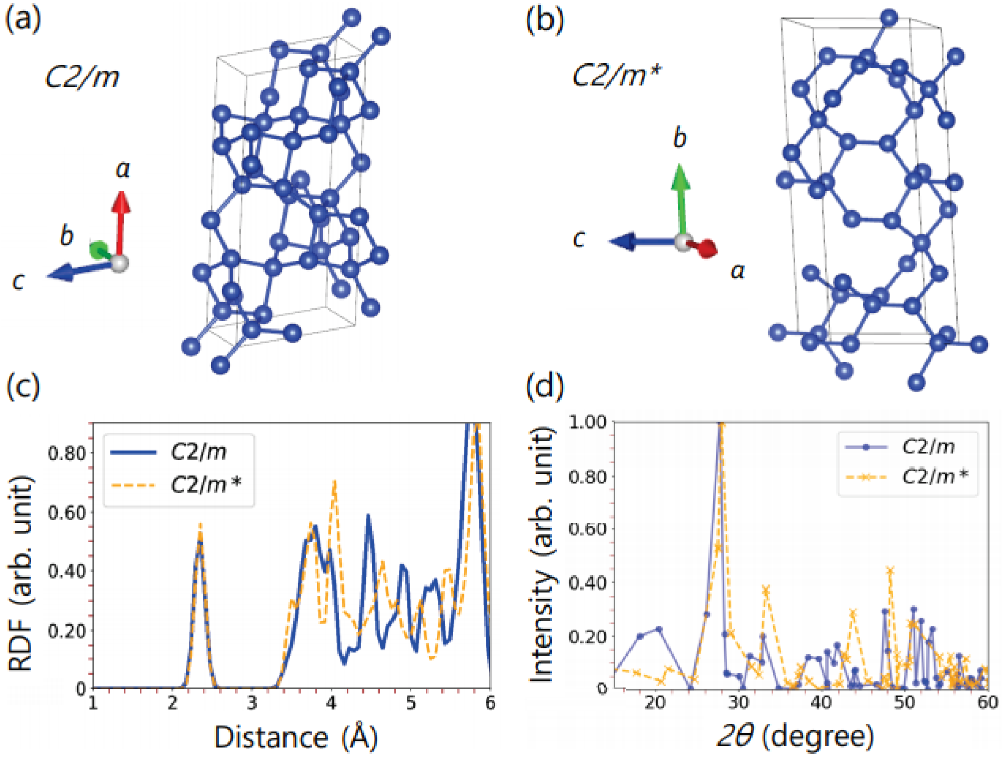


$$r_P = \frac{\sum_{i=1}^{m}(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{m}(x_i - \bar{x})^2}\,\sqrt{\sum_{i=1}^{m}(y_i - \bar{y})^2}}$$

https://github.com/inholeegithub/winter2022

Comput. Mat. Sci. **194**, 110436 (2021).





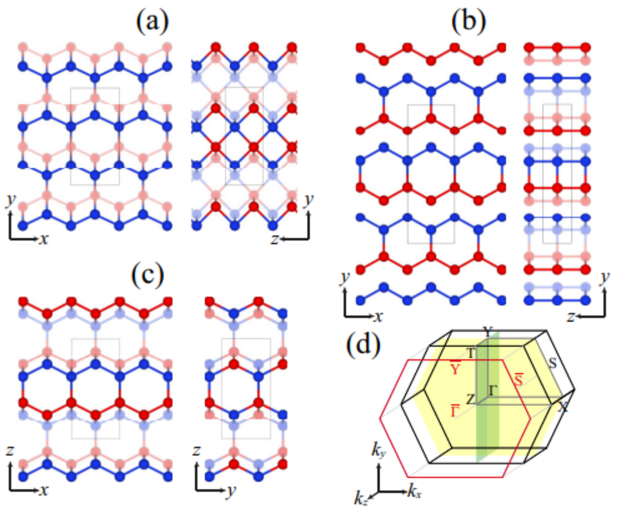
Pearson’s distance between *C2/m* and *C2/m = 0.102**
***C/2m** > C/2m*, 40 meV/atom**
***C2/m* : 2.28 g/cm^3, 0.13 eV**
***C2/m** : 2.39 g/cm^3, 0.28 eV**
Microexplosion experiment*: t32, t32*, m32, m32 [~ BC8]**
***C2/m** is stable by 3-10 meV/atom than these four phases.**

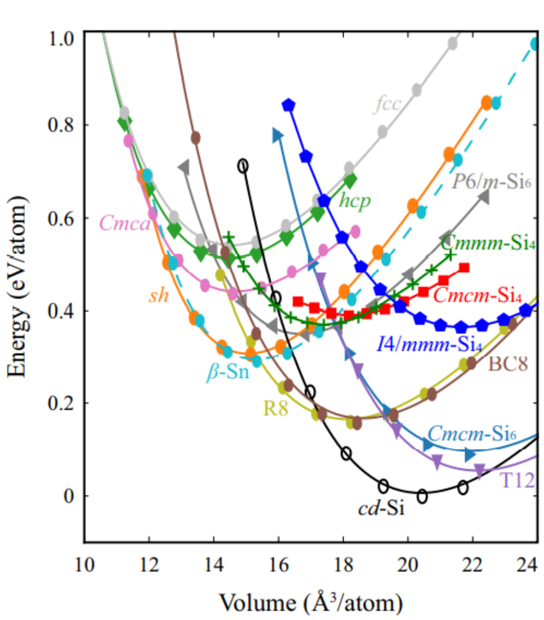
Table 1: Lattice parameters and Wyckoff positions for three Si allotropes, *Cmmm*-Si, *C*2/*m*-Si, and *C*2/*m**-Si.

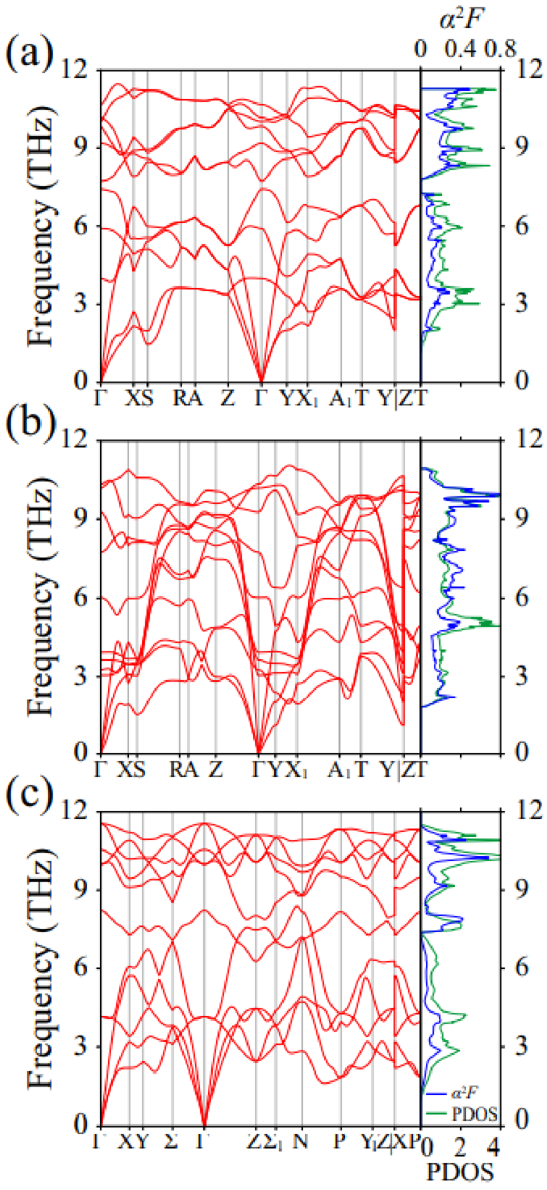
Allotrope	*a* (Å)	*b* (Å)	*c* (Å)	*α* (°)	*β* (°)	*γ* (°)	Wyckoff positions
Cmmm-Si	8.21	6.59	5.20	90.0	90.0	90.0	4 l mm2 (0, 0.50000, 0.75536)
							8 m ..2 (0.25000, 0.25000, 0.72747)
							4 g 2mm (0.86311, 0.00024, 0.99999)
*C*2/*m*-Si	13.73	3.82	6.29	90.0	83.3	90.0	4 i m (0.94460, 0, 0.87347)
							4 i m (0.44097, 1.00000, 0.65322)
							4 i m (0.78744, 0, 0.05727)
							4 i m (0.27303, 1.00000, 0.58547)
*C*2/*m**-Si	3.77	16.56	6.93	90.0	133.7	90.0	4 i m (0.08137, 0, 0.86120)
							8 j 1 (0.07598, 0.87869, 0.36283)
							4 g 2 (0.00029, 0.29131, 0.00058)

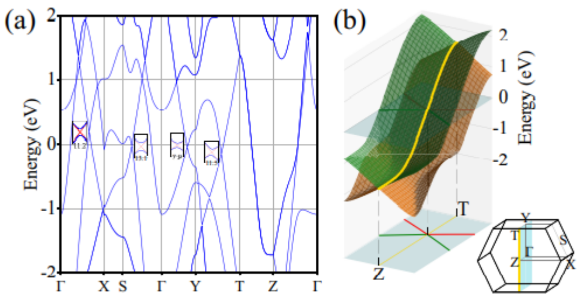
Nat. Commun. **6**, 7555 (2015).
Comput. Mat. Sci. **194**, 110436 (2021).

Ab initio prediction of topological superconductivity in metallic Si allotropes









Allotrope	C_{11}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}	C_{12}	C_{13}	C_{23}
Cmcm-Si_4	147.10	119.16	109.73	33.59	8.02	33.58	60.97	63.10	8.92
Cmmm-Si_4	205.60	145.33	300.06	26.29	69.00	26.46	77.07	−3.59	25.81
I4/mmm-Si_4	108.73	108.73	140.78	36.93	36.93	36.23	68.13	40.17	40.17

Allotrope	Pressure (GPa)	V (Å^3/atom)	$N(0)$ (states/Ry/atom/spin)	λ	$\omega_{\log}$ (K)	T_c (K)
sh-Si	15	13.50	2.44	0.660	250	7.9
P6/m-Si_6	0	16.80	2.40	0.799	263	12.2
Cmcm-Si_4	0	18.18	1.87	0.462	253	2.2
Cmmm-Si_4	0	17.38	2.52	0.808	238	11.4
I4/mmm-Si_4	0	21.64	1.87	0.417	234	1.2

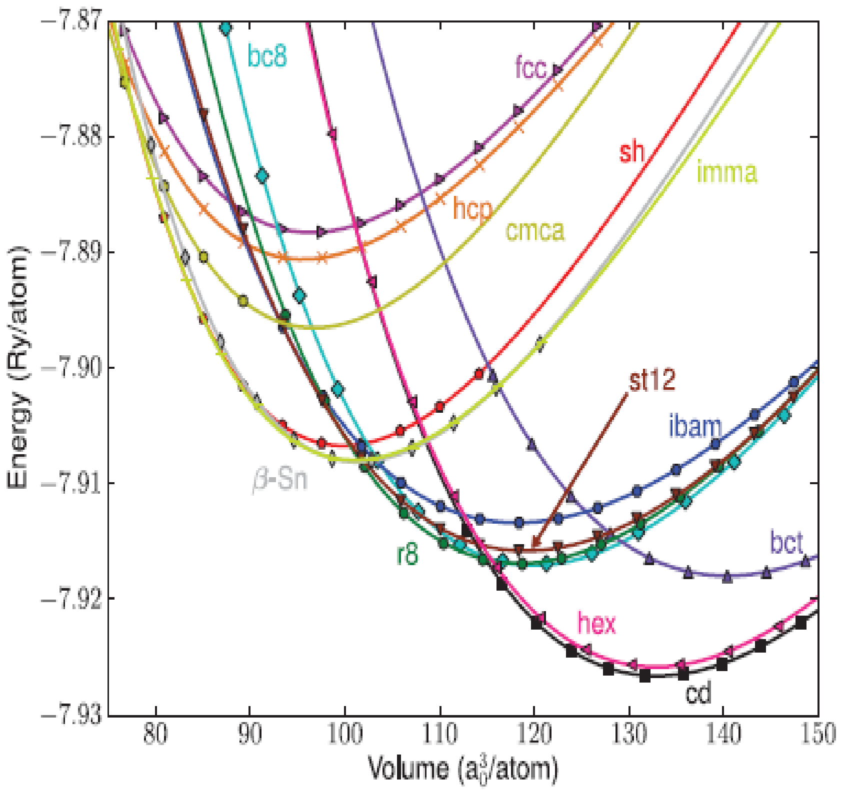
Phys. Rev. Mat. **5**, 104802 (2021).

Contents

- Background {artificial intelligence}
- Evolutionary learning
- Artificial neural networks
- Applications
- [RDFSEARCH, AMADEUS]

Reported crystalline phases of Si under pressure

Si-I (cubic diamond)
Si-II (β-Sn) : metal
Si-III (BC8) : narrow gap
Si-IV (hexagonal diamond)
Si-V (simple hexagonal) : metal
Si-VI (*Cmca*-Si) : metal
Si-VII (hcp) : metal
Si-VIII : not identified yet
Si-IX : not identified yet
Si-X (fcc) : metal
Si-XI (*Imma*-Si) : metal
Si-XII (R8) : indirect gap 0.24 eV
Si-XIII (T12) : indirect gap
BT8, ST12 : indirect gap
clathrates (type-I, type-II), *Cmcm*-Si_6

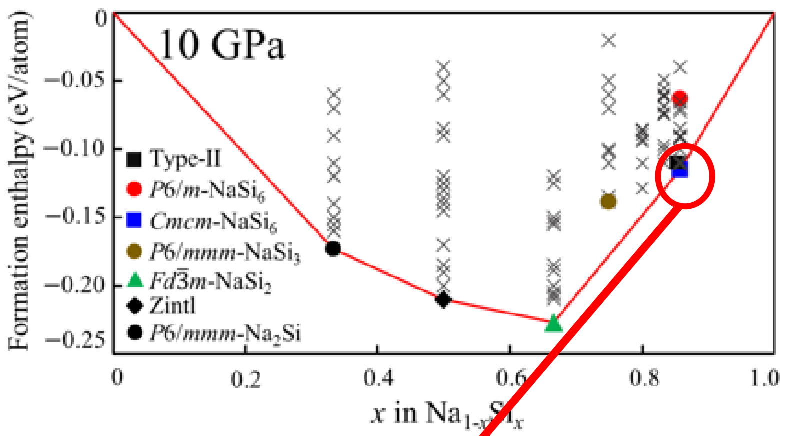


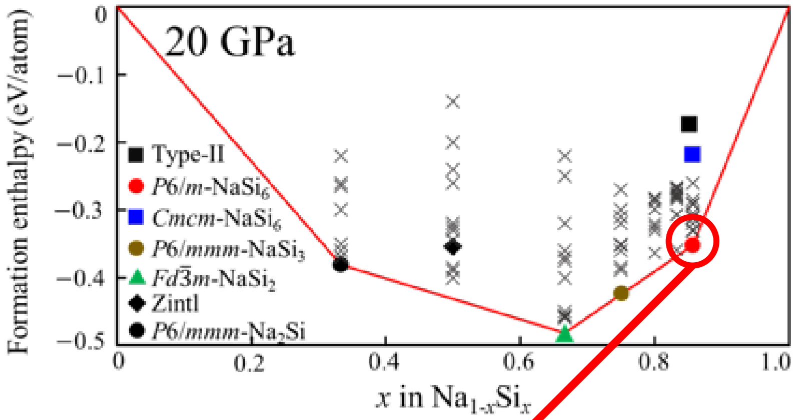
B.D. Malone, M.L. Cohen, Phys. Rev. B (2012).

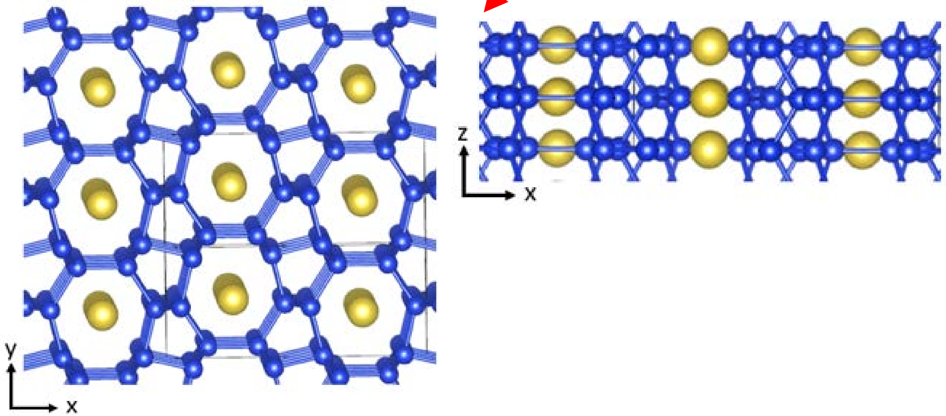
- **Si allotropes with direct band gaps have not been synthesized.**
- **High pressure metallic phases (β-Sn, sh, hcp, fcc) do not maintain their crystal structures after pressure release.**
- **Metallic Si phases at ambient pressure had not been reported before April 11, 2018.**

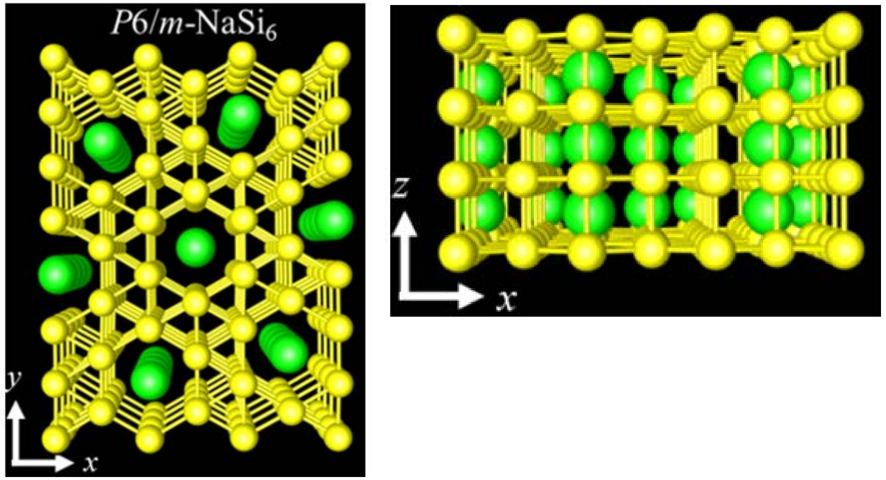
Phys. Rev. Lett. **120**, 157001 (2018).

$NaSi_6$ clathrate at high pressure









- ***Cmcm*-$NaSi_6$ at 10 GPa**

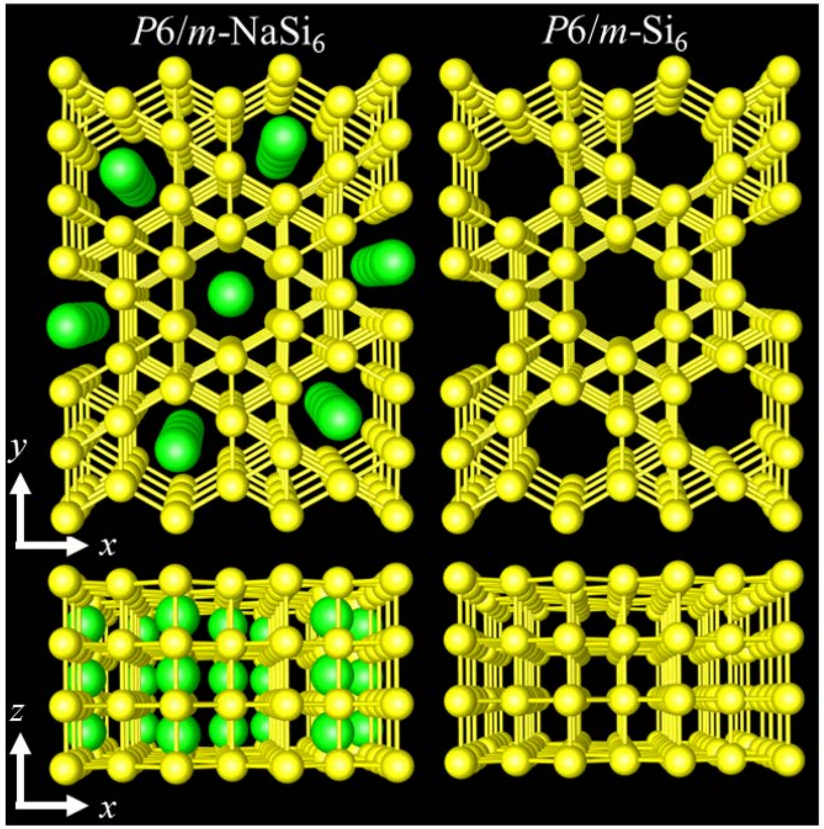
[Cryst. Growth Des. **13**, 303 (2013)]

- ***P6/m*-$NaSi_6$ at 20 GPa**
- **Transition pressure from *Cmcm*-$NaSi_6$ to *P6/m*-$NaSi_6$: 12.4 GPa**

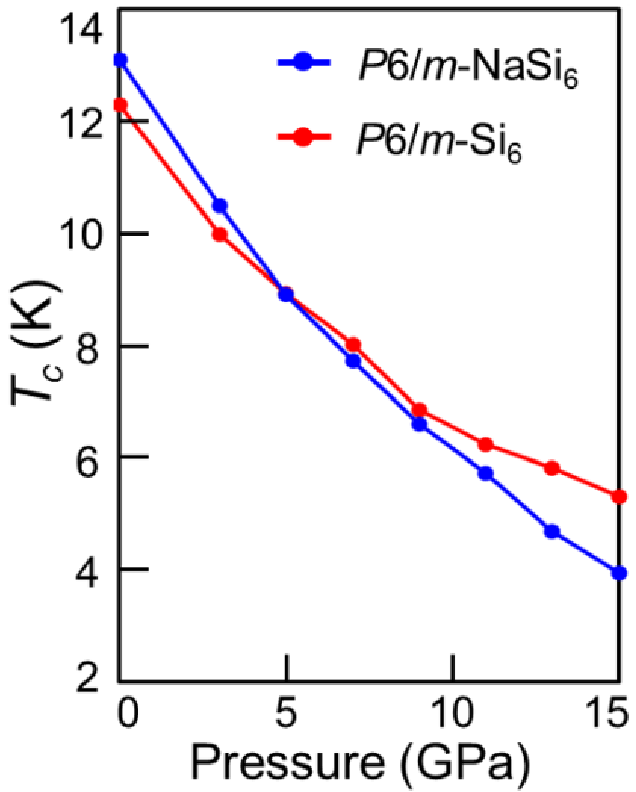
Phys. Rev. Lett. **120**, 157001 (2018).

Superconducting *P6/m*-$NaSi_6$ and *P6/m*-Si_6 clathrates

(first proposed)



Pressure dependence of T_c



- ➢ ***P6/m*** **space group**
- ➢ **Simple hexagonal with open channels**
- ➢ **Na atoms along open channels**
- ➢ **Stable at ambient pressure**
- ➢ **Metallic**

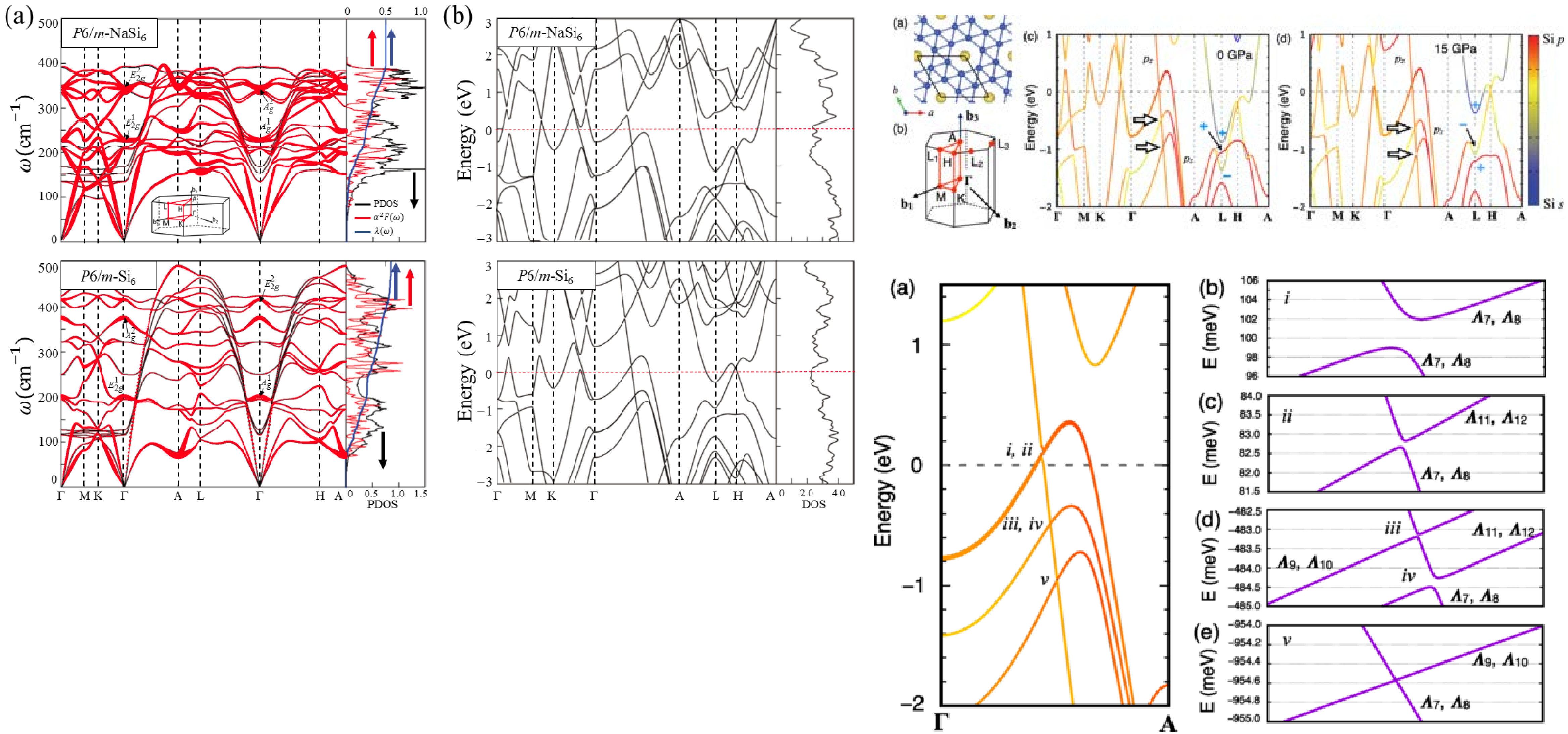
➢ **Superconducting at ambient pressure**

- T_c = 13.1 K for *P6/m*-$NaSi_6$
- T_c = 12.2 K for *P6/m*-Si_6

Phys. Rev. Lett. **120**, 157001 (2018); Phys. Rev. B **107**, 115127 (2023).

KRISS

$Na_{1-x}Si_x$



Phys. Rev. Lett. **120**, 157001 (2018); Phys. Rev. B **107**, 115127 (2023).

A new superconducting open-framework allotrope of silicon at ambient pressure

Allotrope	Pressure (GPa)	V (Å³/Si-atom)	$N(0)$ (states/Ry/Si-atom/spin)	λ	$\omega_{\log}$ (K)	T_c (K)
$P6/m$-$NaSi_6$	0	18.4	2.82	0.897	225	13.1
	15	16.1	2.60	0.498	331	4.0
$P6/m$-Si_6	0	16.8	2.40	0.799	263	12.2
	15	14.8	2.22	0.556	299	5.3
sh-Si	15	13.5	2.44	0.660	250	7.9

T_c=4–8 K
high-pressure β-Sn phase of Si,
high-pressure *sh* phase of Si,
type-I clathrate of $(Na, Ba)_x$-Si_{46},
Ba_8Si_{46}

Phys. Rev. Lett. **120**, 157001 (2018); Phys. Rev. B **107**, 115127 (2023).

KRISS

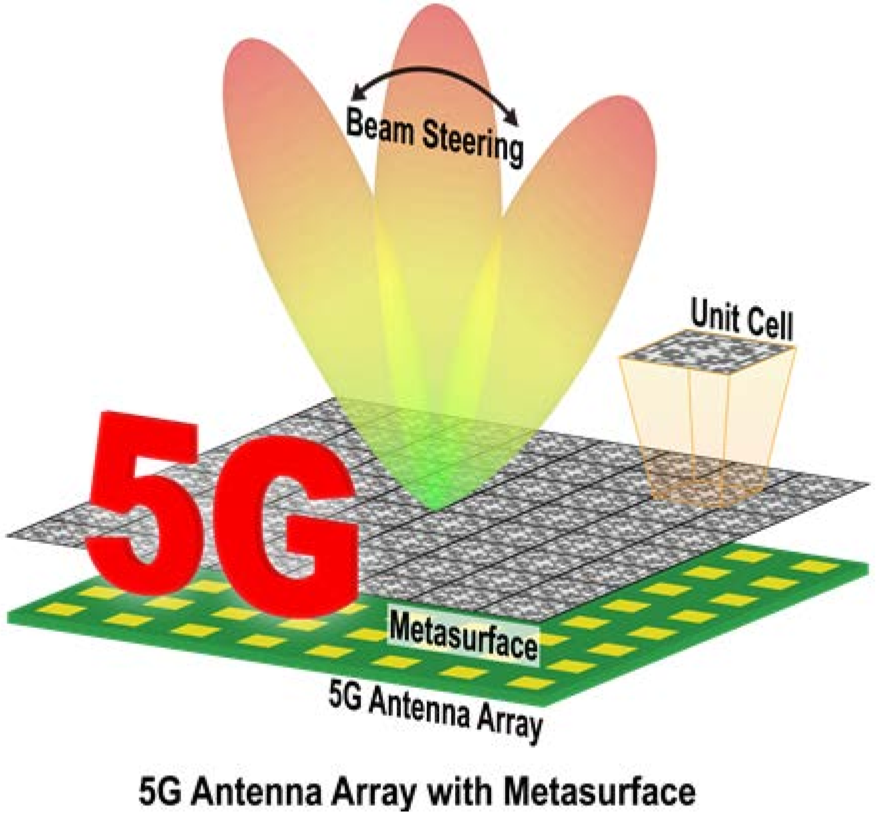
Design of single-layer metasurface filter by CSA for 5G mm-wave communications

It is anticipated that 28 GHz and 38 GHz mmWave bands will play a key role in 5G deployments and beyond-5G systems.
[pre-assigned frequency response characteristic functions required in the 5G frequency band]
[low in-band loss and high out-of-band suppression] [the widest bandwidth]
[angular stability] [polarization insensitivity]

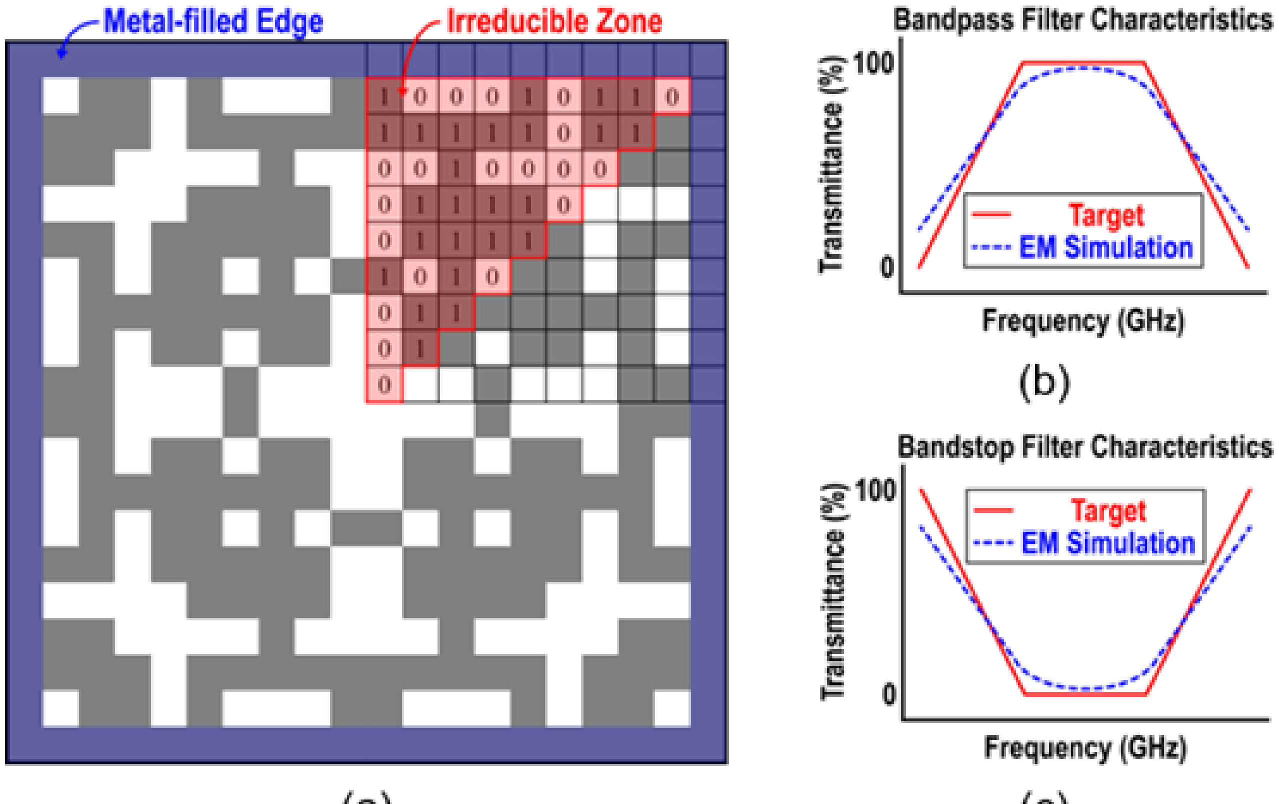
The more pixels the better.

Objective function

$$f(\vec{x}) = \sum_{k=1}^{N} | T_{target}(\nu_k) - T_{EM}(\nu_k;\vec{x}) | .$$



Coexistence of 5G With Fixed Satellite Service at 28 GHz

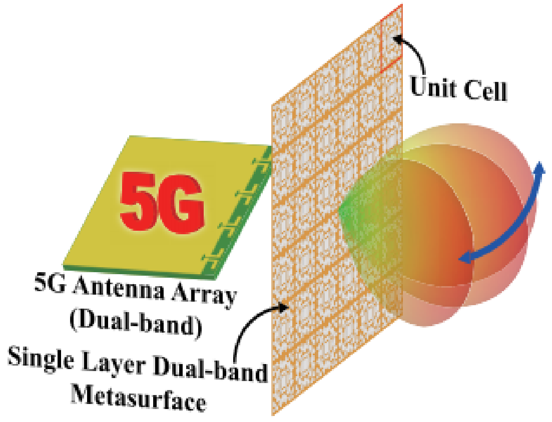


(a)

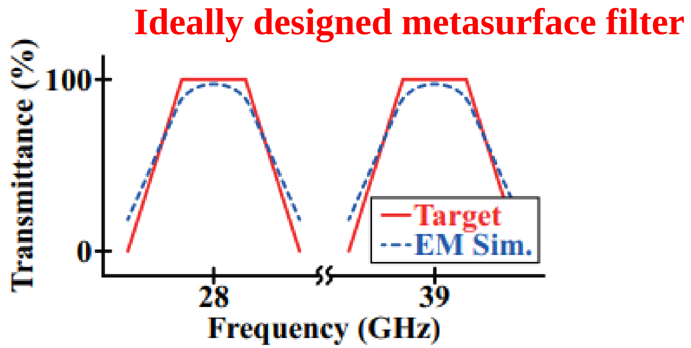
50 μm thick flexible polyethylene terephthalate film
6 μm thick copper foil

IEEE Access **9**, 29764 (2021); Appl. Phys. Lett. **119**, 174101 (2021); License-out

Design of dual-band single-layer metasurfaces for millimeter-wave 5G communication systems



5G Antenna Array with Metasurface



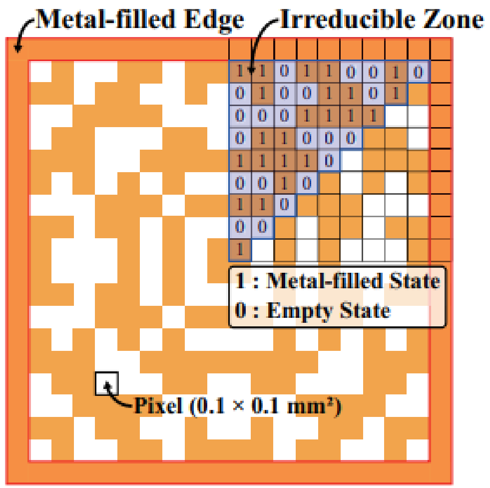
Dual Band-pass Filter Characteristic

Objective function

$$f(\vec{x}) = \sum_{k=1}^{N} \left| T_{target}(\nu_k) - T_{EM}(\nu_k;\vec{x}) \right| .$$

generic flexible single-layer pixel-based unit-cell

50 µm
6 µm



Unit Cell Structure ($n \times n$ pixels)

Transmittance of the surface of a material is its effectiveness in transmitting radiant energy. It is the fraction of incident electromagnetic power that is transmitted through a sample, in contrast to the transmission coefficient, which is the ratio of the transmitted to incident electric field.

Approaches reported in the literature, which can be classified into three types of dual-band solutions—multilayer metasurfaces, fractal elements, and multi-resonant metasurfaces—have been utilized for enabling interference alleviation techniques. Typical metasurfaces rely on the introduction of multiple resonators that resonate separately by frequency.

https://en.wikipedia.org/wiki/Transmittance

IEEE Access **9**, 29764 (2021); Appl. Phys. Lett. **119**, 174101 (2021); License-out

The **decibel** (symbol: **dB**) is a relative unit of measurement equal to one tenth of a **bel** (**B**).

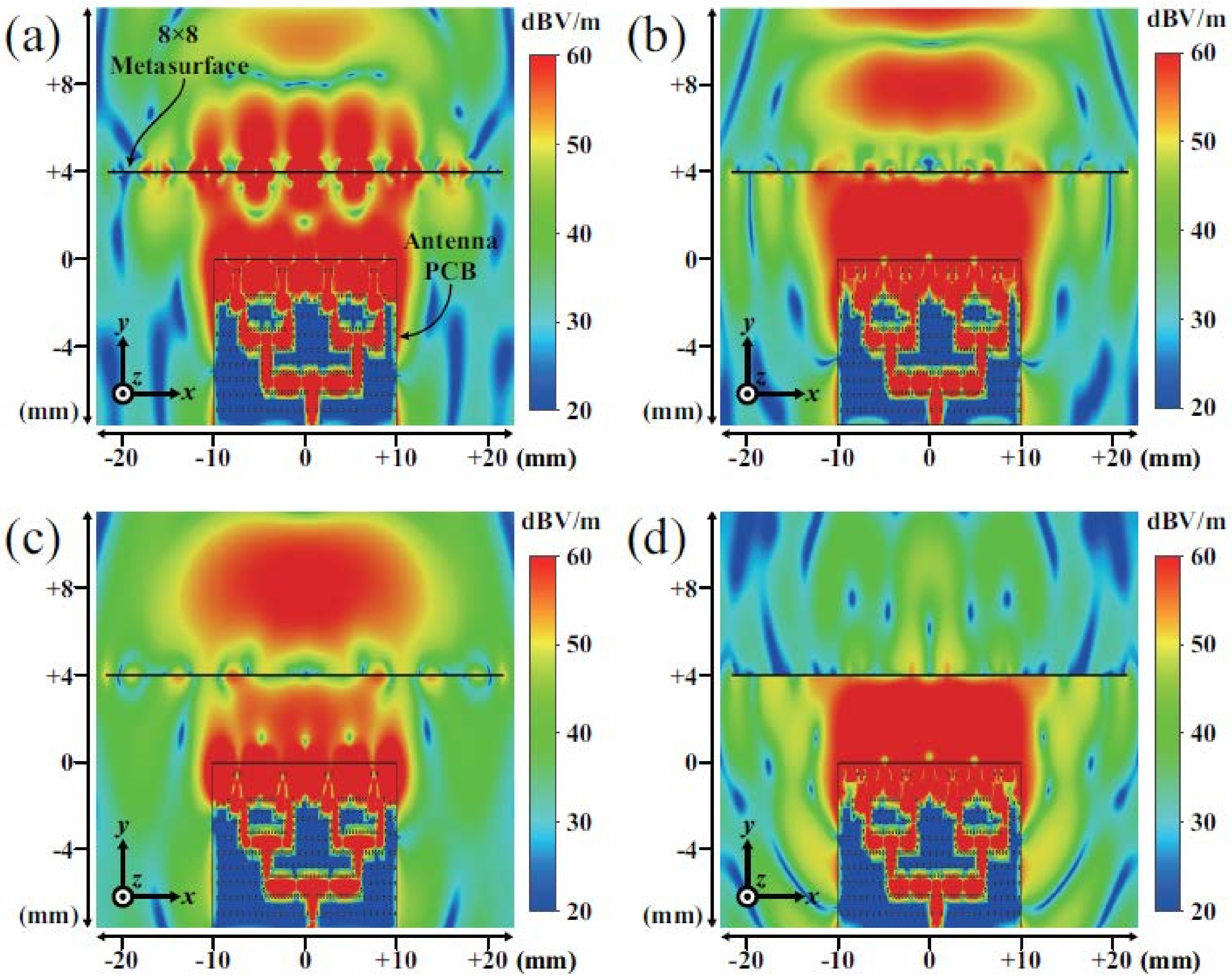
Table: Gain / loss in decibels

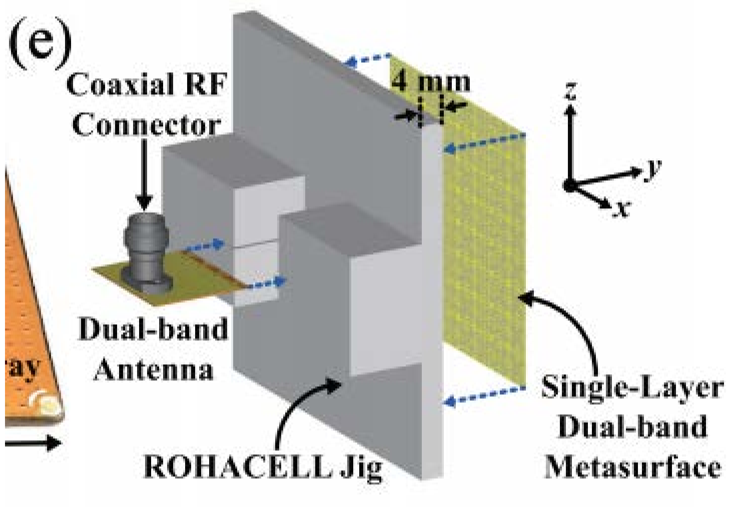
Loss/gain as a ratio	Loss/gain in decibels	Loss/gain as a ratio	Loss/gain in decibels
$\frac{P_{output}}{P_{input}}$	$10 \log \frac{P_{output}}{P_{input}}$	$\frac{P_{output}}{P_{input}}$	$10 \log \frac{P_{output}}{P_{input}}$
1000	30 dB	0.1	-10 dB
100	20 dB	0.01	-20 dB
10	10 dB	0.001	-30 dB
1 (no loss or gain)	0 dB	0.0001	-40 dB

https://www.youtube.com/watch?v=4vw6wVP81No&list=PLTIv6N2kNYZamqDqPdGSBDN1Gc6rW-KET&index=11

https://en.wikipedia.org/wiki/Decibel

Simulated electric field intensity distributions
(x-component of electric field) of prototype configurations.
5G antenna array with 28/39 GHz dual BPF
at (a) 29.5 GHz (passband) and (b) 39.0 GHz (passband).
5G antenna array with 28 GHz BFP/39 GHz BSF
at (c) 27.0 GHz (passband) and (d) 39.0 GHz (stop band).





Appl. Phys. Lett. **119**, 174101 (2021); License-out

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- Background {artificial intelligence}
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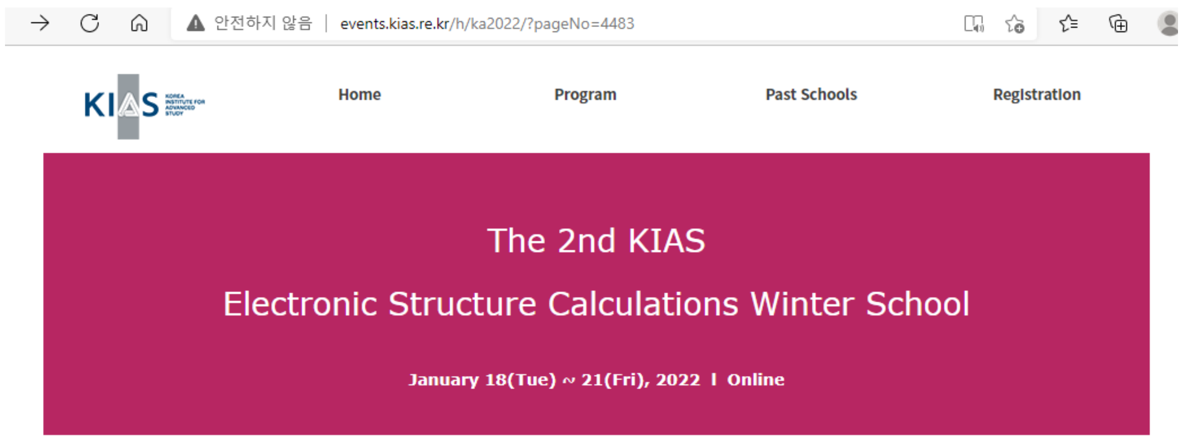
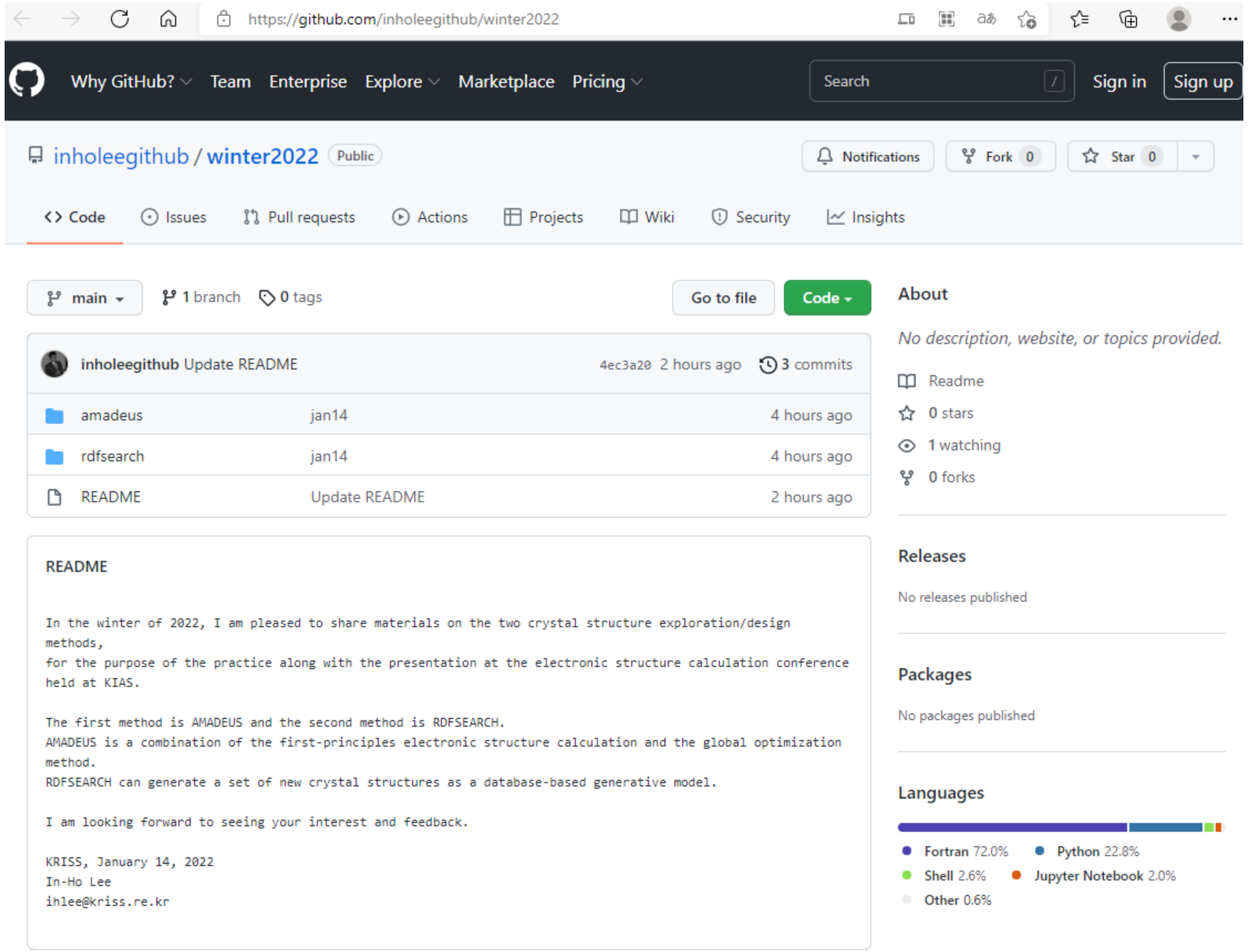
- [RDFSEARCH, AMADEUS]

- http://events.kias.re.kr/h/ka2022/?pageNo=4483
- https://github.com/inholeegithub/winter2022



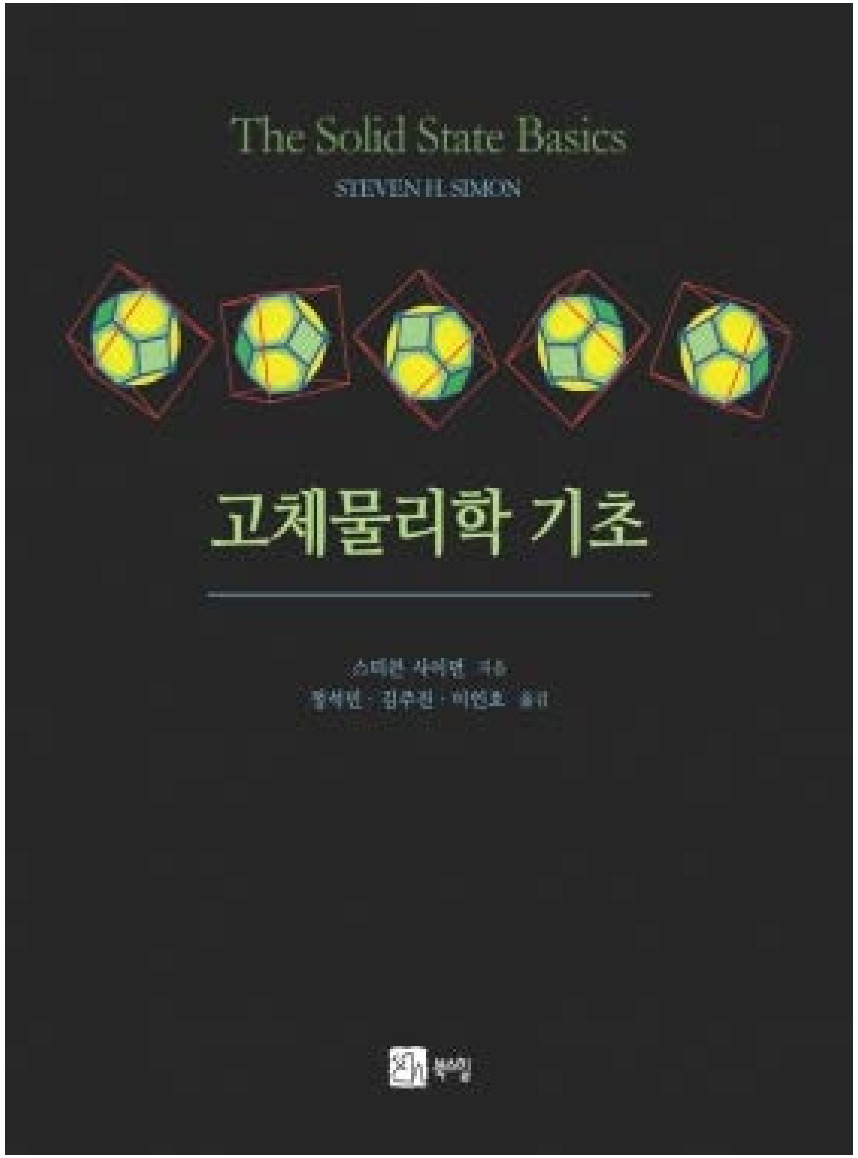


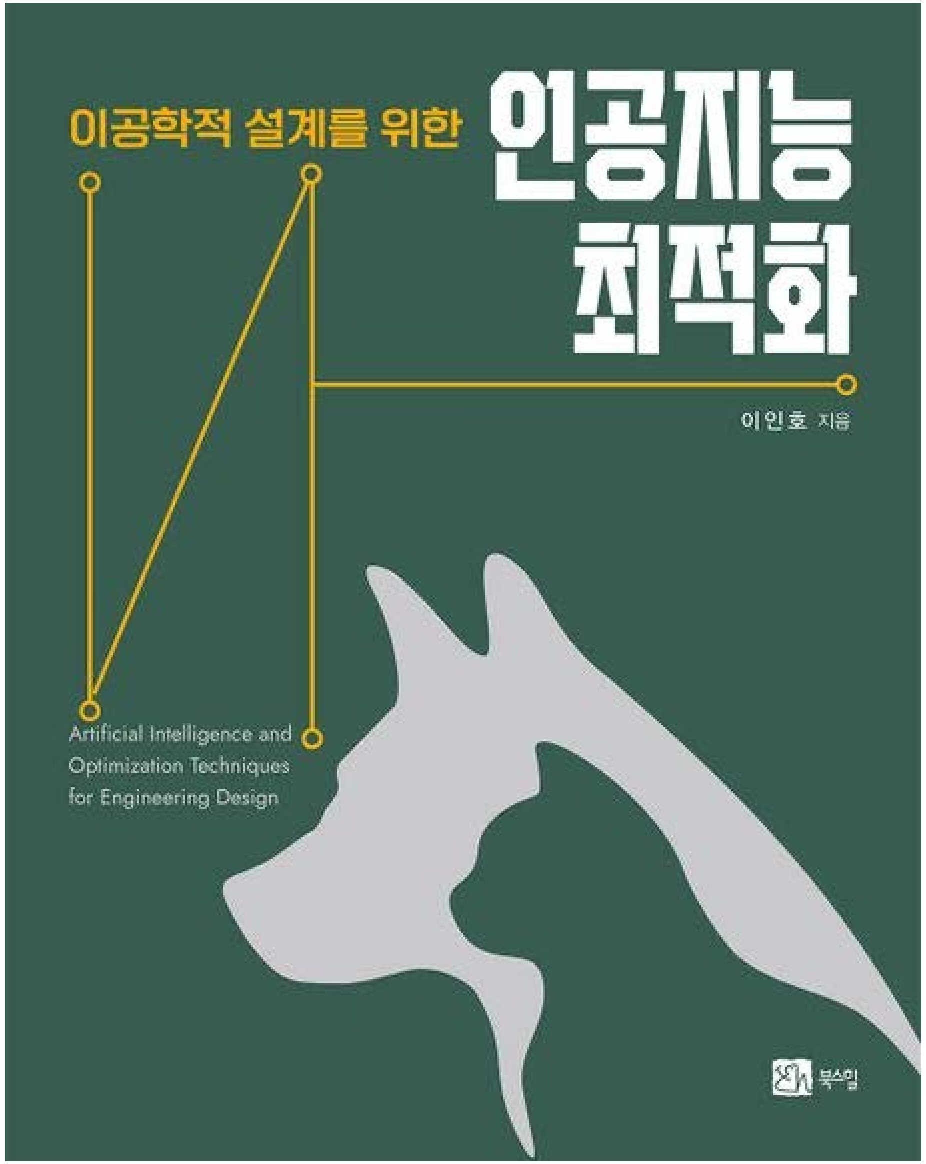
강사: 이인호 박사(KRISS) 1/2 _ 제2회 KIAS 전자구조계산 겨울학교 - YouTube

강사: 이인호 박사(KRISS) 2/2 _ 제2회 KIAS 전자구조계산 겨울학교 - YouTube

Conclusions

- Conformational Space Annealing (CSA)
- AMADEUS (many applications)
- Action-CSA (reaction path search)
- Replica RDFs (VAE)
- Solar cell (Si)
- LED (C)
- High-mobility (P)
- Topological materials (Si, C, $Ag_2Se_{0.5}Te_{0.5}$)
- Topological superconductivity (Si)
- Structural searches (2D, 3D types of B)
- Metasurfaces for 5G communication systems (License-out)


The Solid State Basics
STEVEN H. SIMON
고체물리학 기초
스티븐 사이먼 지음
북스힐


이공학적 설계를 위한
인공지능 최적화
이인호 지음
Artificial Intelligence and
Optimization Techniques
for Engineering Design
북스힐