Φ – 575 Διάλεξη 01

Φυσική διατάξεων δισδιάστατων ημιαγωγών

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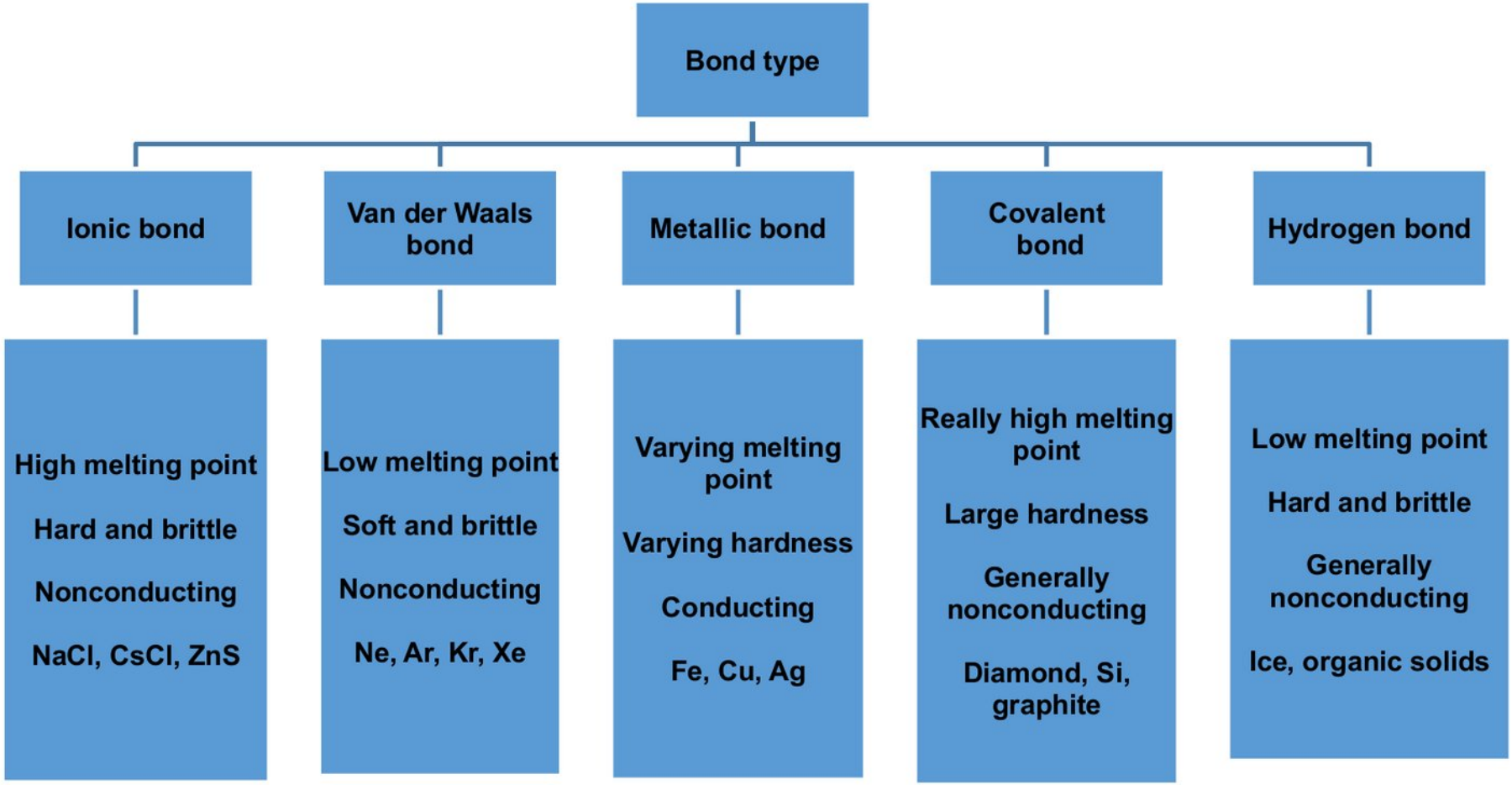
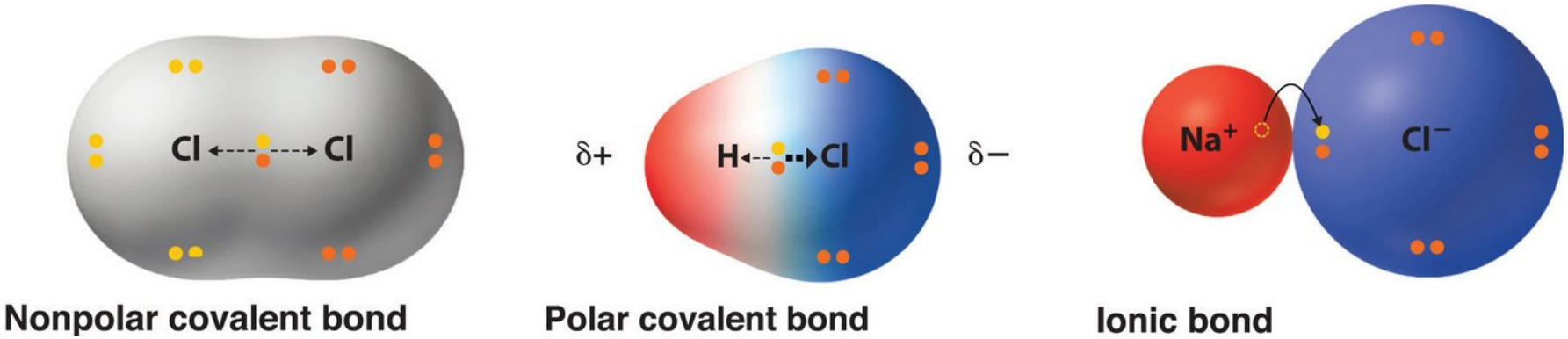
Είδη δεσμών κ χαρακτηριστικά τους



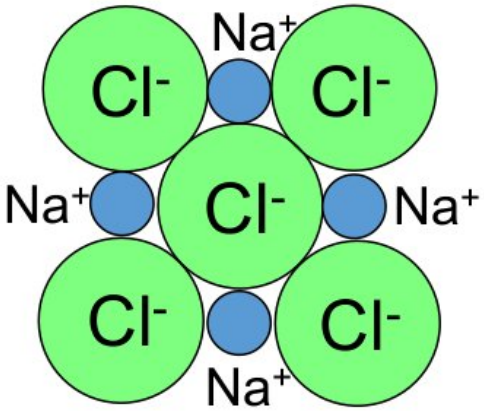
Ημιπολικός δεσμός

Ομοιοπολικός δεσμός υπάρχει μόνο μεταξύ όμοιων ατόμων.
Μεταξύ ανόμοιων ατόμων υπάρχει κάποιος βαθμός πολικότητας (ιοντικός χαρακτήρας)

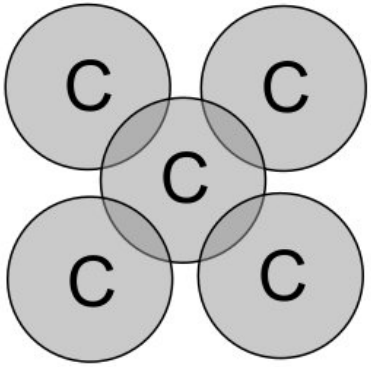


Ιοντικός – Ομοιοπολικός δεσμός

Ιοντικός δεσμός: Ηλεκτρόνια μεταφέρονται από το ενα ατομο στο αλλο
Ομοιοπολικός δεσμός: Ηλεκτρόνια διαμοιράζονται μεταξύ ατόμων σε γειτονία



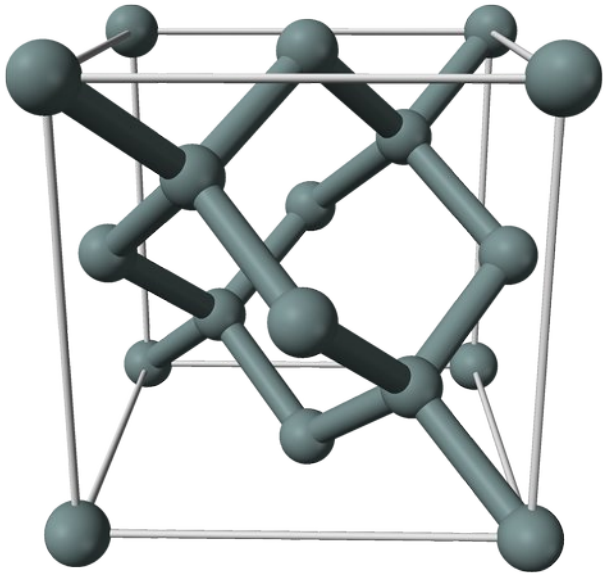
Sodium chloride (ionic)

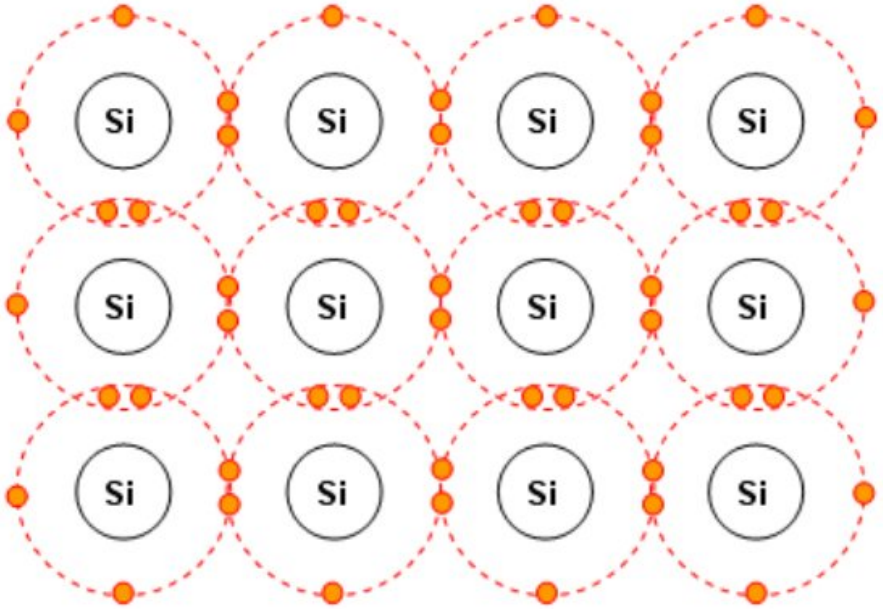


Diamond (covalent)

Παραδειγμα δεσμού

Ηλεκτρόνιακή δομή Si: $1s^2 2s^2 2p^6 3s^2 3p^2$
4 ηλεκτρόνια ζώνη σθένους, 4 ηλεκτρόνια λείπουν για να συμπληρωθεί η στοιβάδα

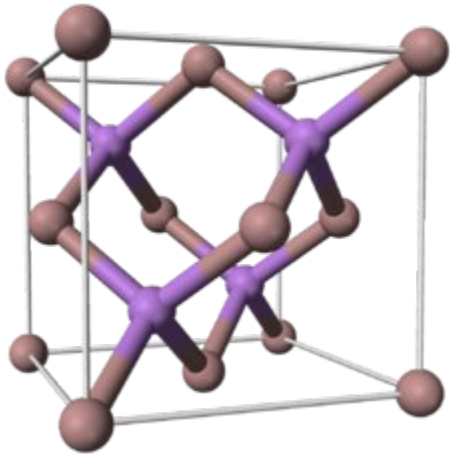


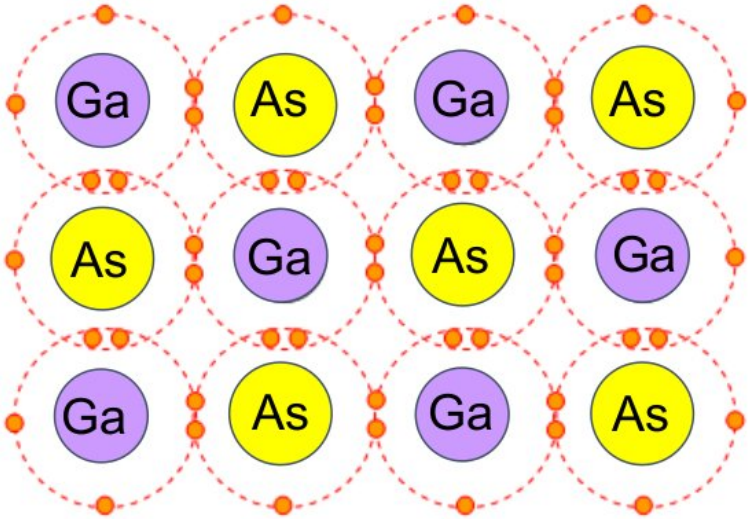


Τι δεσμός είναι αυτός?

Παραδειγμα 2

Ηλεκτρόνιακή δομή Ga: $1s^2 2s^2 2p^6 3s^2 p^6 3d^{10} 4s^2 4p^1$
3 ηλεκτρόνια ζώνη σθένους, 5 ηλεκτρόνια λείπουν για να συμπληρωθεί η στοιβάδα
Ηλεκτρόνιακή δομή As: $1s^2 2s^2 2p^6 3s^2 p^6 3d^{10} 4s^2 4p^3$
5 ηλεκτρόνια ζώνη σθένους, 3 ηλεκτρόνια λείπουν για να συμπληρωθεί η στοιβάδα

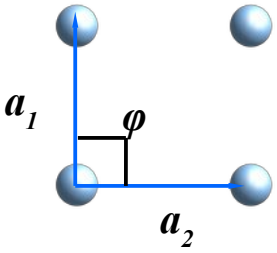




Τι δεσμός είναι αυτός?

Τύποι 2D κρυστάλλων (Bravais)

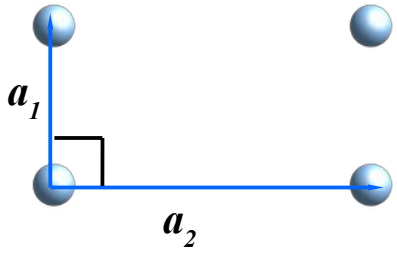
Square lattice



$|a_1| = |a_2|$

$\varphi = 90\,^\circ$

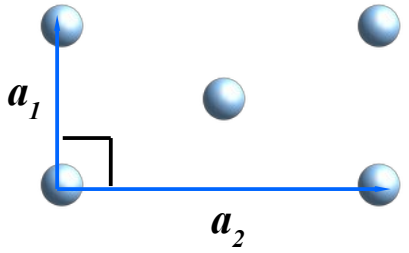
Rectangular lattice



$|a_1| \neq |a_2|$

$\varphi = 90\,^\circ$

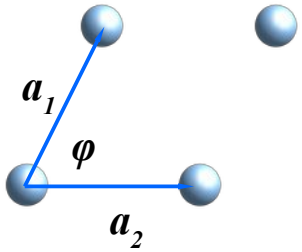
Centered rectangular lattice



$|a_1| \neq |a_2|$

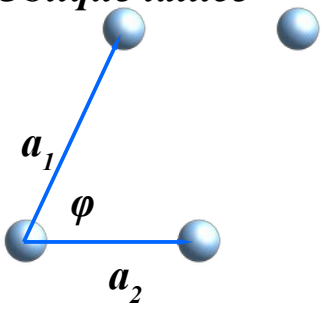
$\varphi = 90\,^\circ$

Hexagonal lattice



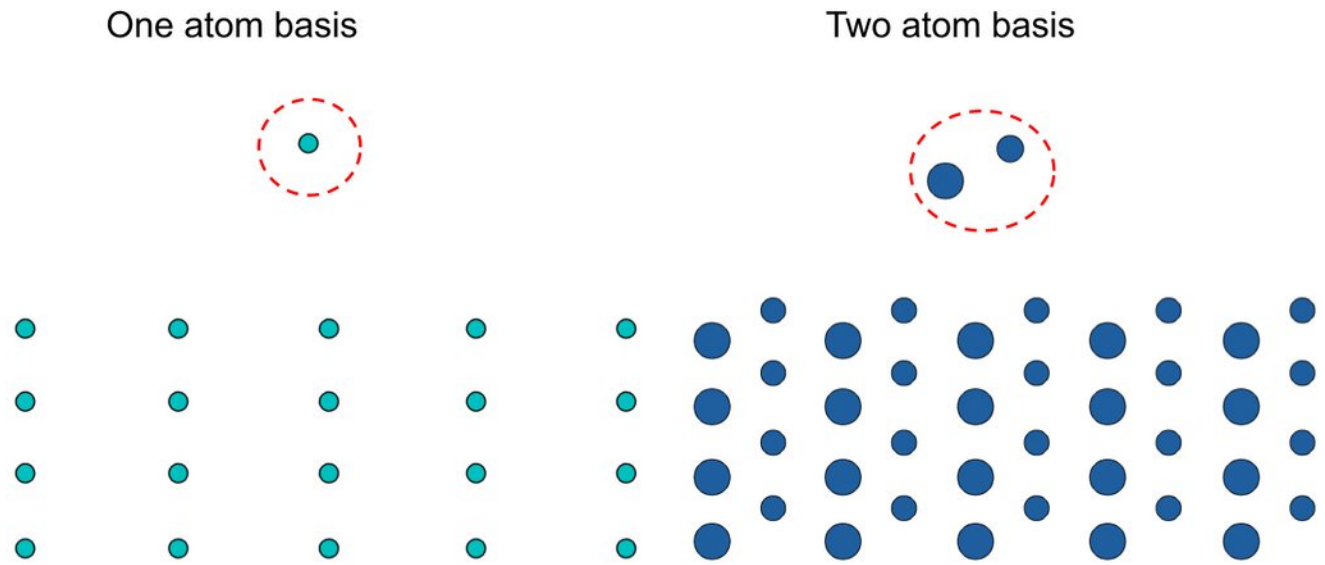
$|a_1| = |a_2|$ $\varphi = 60\,^\circ$

Oblique lattice



$|a_1| \neq |a_2|$

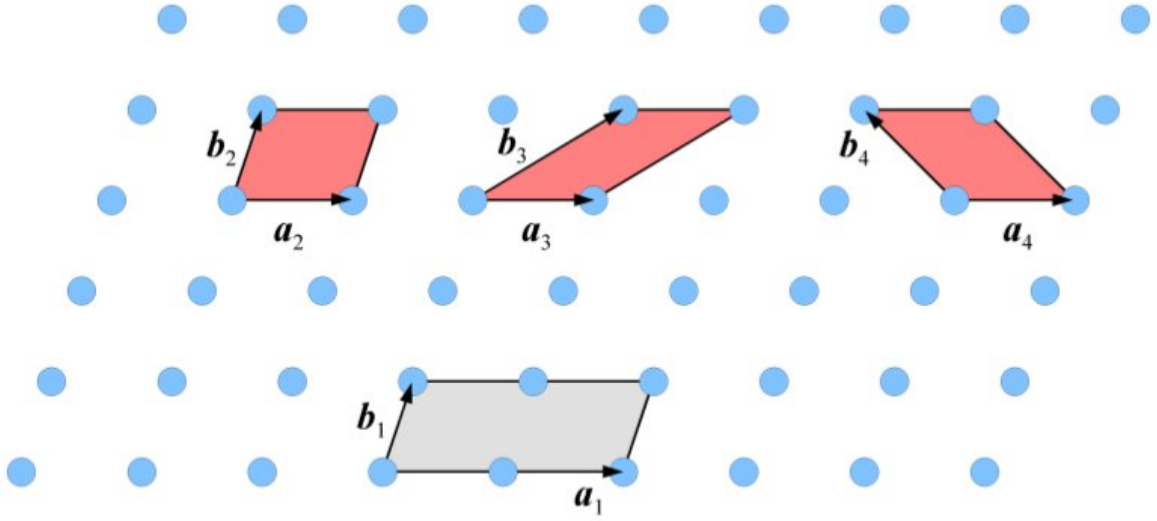
Κρυσταλλοι



Η βάση του κρυστάλλου αποτελείτε από ένα άτομο

Η βάση του κρυστάλλου αποτελείτε από δύο άτομα (εδώ ανόμοια)

Lattice indexing



Αν θεωρήσουμε τα a_2, b_2 ώς διανύσματα αναφοράς τότε:

$$\vec{b}_3 = \vec{a}_2 + \vec{b}_2 \,,\; \vec{a}_3 = \vec{a}_2$$

$$\vec{b}_4 = \vec{a}_2 - \vec{b}_2 \,,\; \vec{a}_4 = \vec{a}_2$$

$$\vec{b}_1 = \vec{b}_2 \,,\; \vec{a}_1 = 2 \times \vec{a}_2$$

Συμμετρίες (2D Laue classes)

In two dimensions there are (besides identity): mirror, rotation, and glide

In 2D, six crystallographic point groups (2D Laue classes) are compatible with lattice periodicity:

1)1 (no rotational symmetry beyond identity)

2) 2 (twofold rotation)

3) m (single mirror line)

4) 2mm (twofold rotation + two perpendicular mirror lines)

5) 3m (threefold rotation + mirrors, hexagonal lattice)

6) 4mm (fourfold rotation + mirrors, square lattice)

7) 6mm (sixfold rotation + mirrors, hexagonal lattice)

Another representation comes from applying:
Rotation symmetry (1, 2, 3, 4, 5, 6 fold)
and Mirror and glide operation and combining them to get the SAME Laue classes

Συμμετρία II (περιστροφή)

In two dimensions there are (besides identity): mirror, rotation, and glide

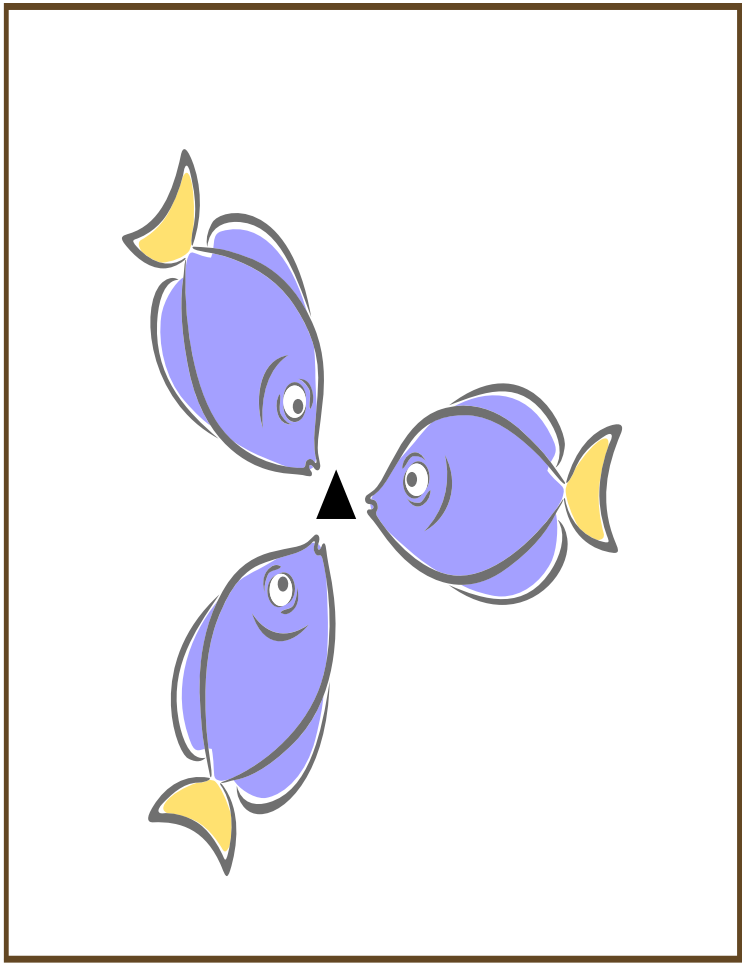


Figure by MIT OpenCourseWare.

Συμμετρία Ι (κατοπτρισμός)

In two dimensions there are (besides identity): mirror, rotation, and glide

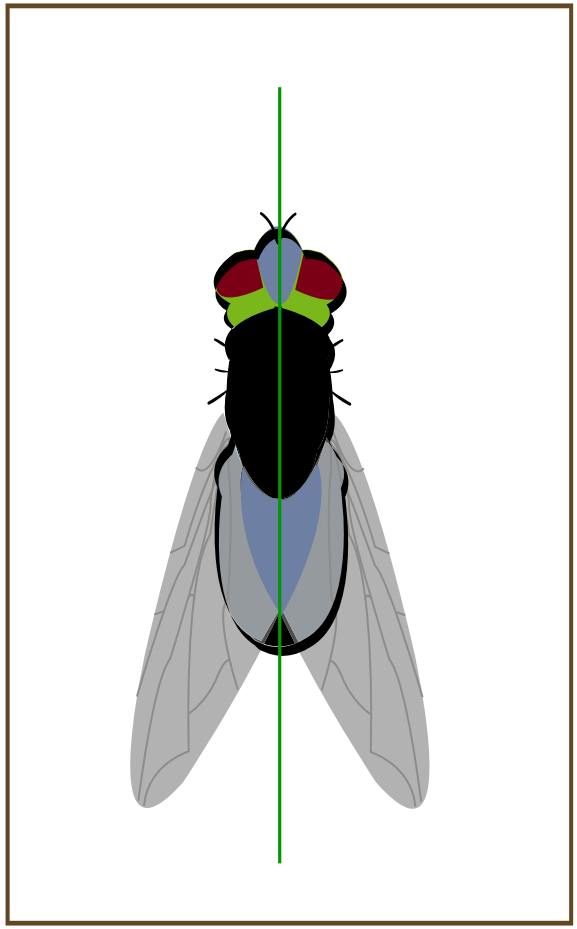


Figure by MIT OpenCourseWare.

Συμμετρία ΙΙΙ (Ολίσθηση)

In two dimensions there are (besides identity): mirror, rotation, and glide

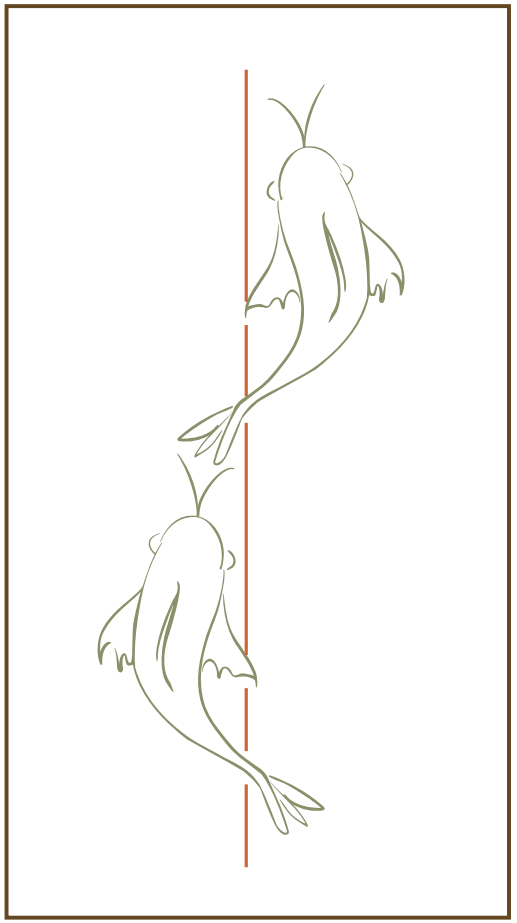


Figure by MIT OpenCourseWare.

Συμμετρία σε 2D υλικα

Combining all the above operations result in 17 symmetry groups

The 17 groups (in international notation) are usually listed as:

Oblique: p1, p2

Rectangular: pm, pg, cm, p2mm, p2mg, p2gg, c2mm

Square: p4, p4mm, p4gm

Hexagonal: p3, p3m1, p31m, p6, p6mm

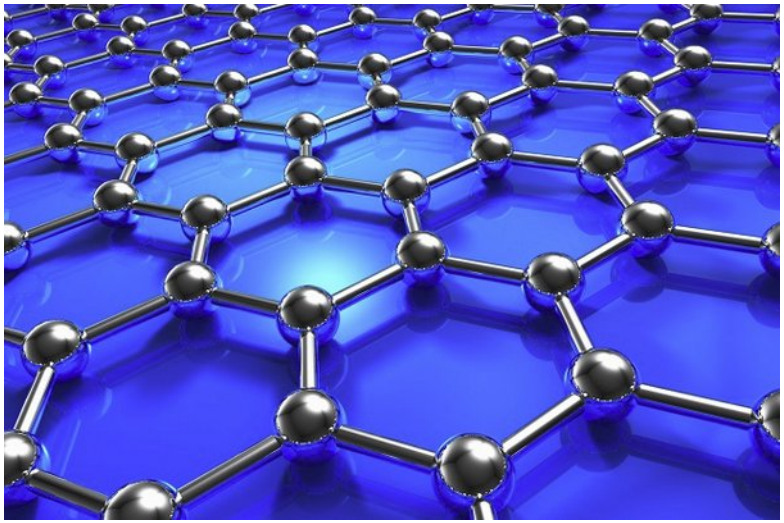
Κατηγορίες συμμετρίας σε 2D υλικά

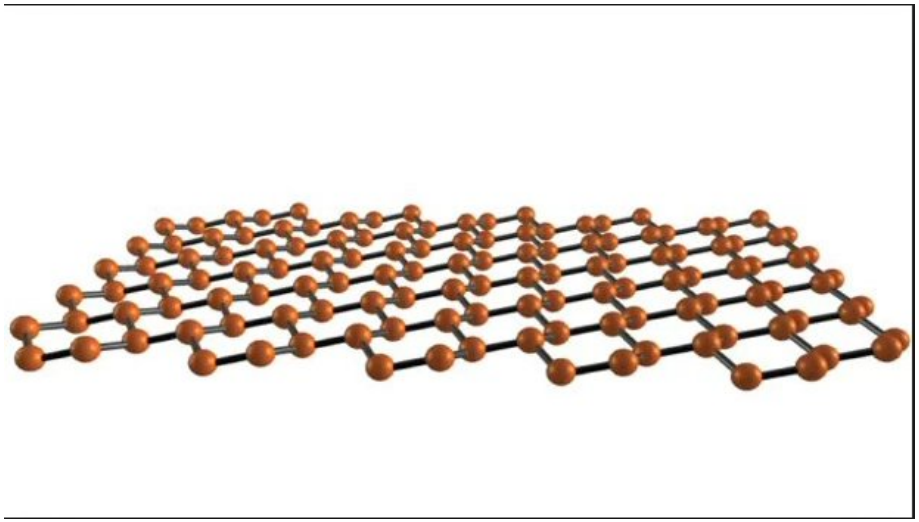
Summary table of main 2D symmetry categories

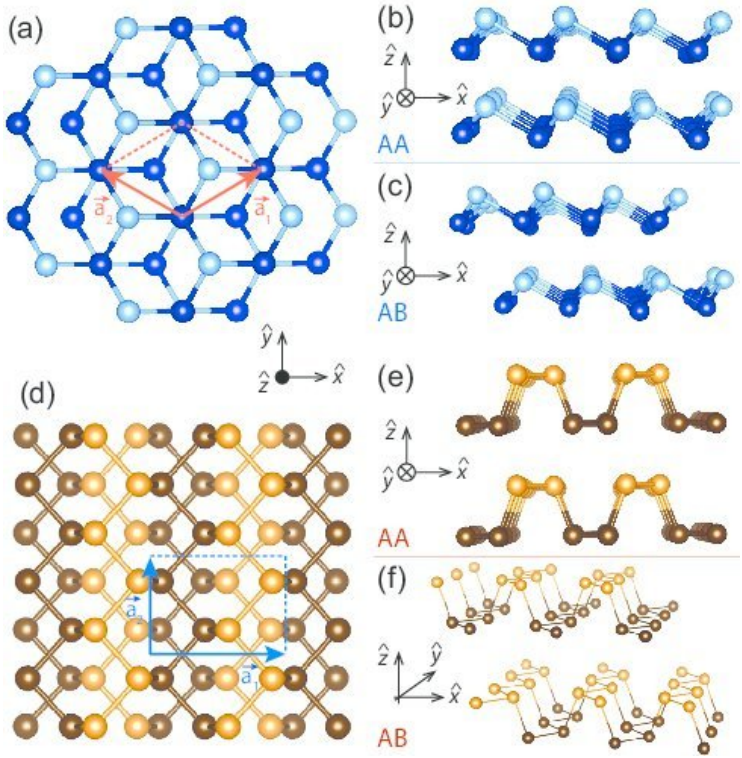
Level	How many?	What they encode	Citations
Bravais lattices	5	Pure translation symmetry of 2D lattice	(Dempsey & Moeck, 2020; Gratias & Quiquandon, 2023; Moeck, 2018)
2D point groups/Laue	6	Rotations + mirrors about a point	(Dempsey & Moeck, 2020; Landsberg & Hankamer, 2007; Moeck, 2018)
Plane (wallpaper) groups	17	Full 2D space-group symmetry of patterns	(Červeň, 2025; Dempsey & Moeck, 2020; Yan, 2024; Landsberg & Hankamer, 2007; Moeck, 2018)

FIGURE 1 Hierarchy of 2D lattice, point, and plane symmetries.

Graphene, Germanene, Silicene e.t.c.

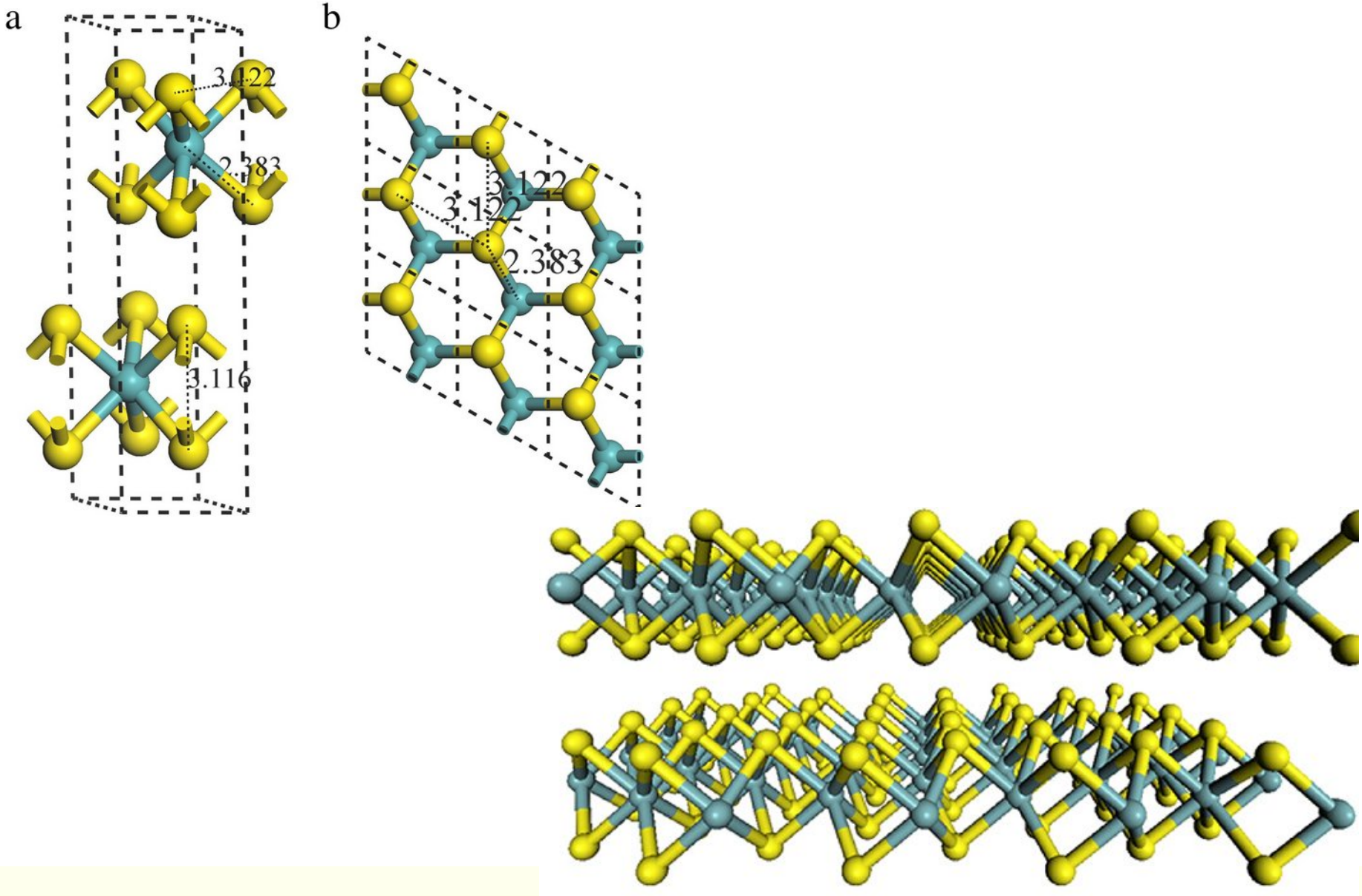






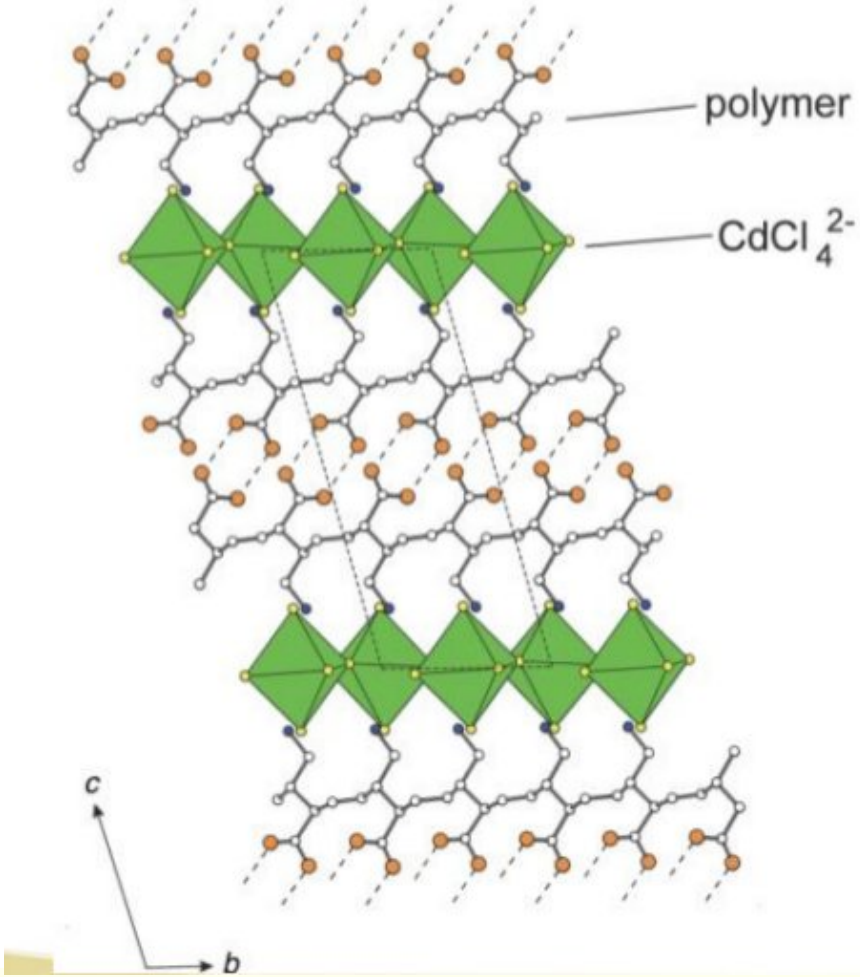
Group theory for structural analysis and lattice vibrations in phosphorene systems May 2015 Physical Review B 91(20)
DOI: 10.1103/PhysRevB.91.205421

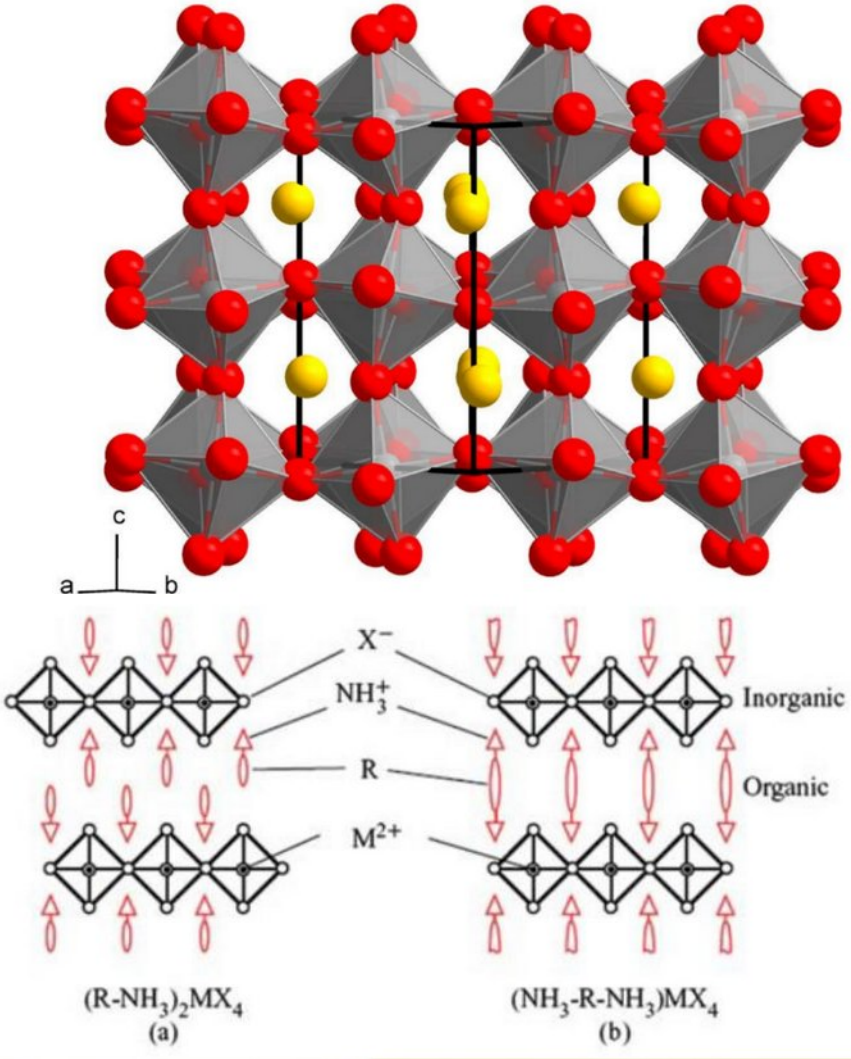
Διχαλκογενίδια



Pseudo 2D Perovskites

6-amino-2,4-trans,trans-hexadienoic acid, within a cadmium (II) chloride perovskite framework





Further reading

- https://ocw.mit.edu/courses/chemistry/5-069-crystal-structure-analysis-spring-2010/lecture-notes/symm_handout1_re.pdf
- www.physics.smu.edu/scalise/P5337fa11/notes/ch03/2DLatticeUnitCell.pdf
- https://en.wikipedia.org/wiki/Crystal_structure
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- 2 / 3Chen, Z., Zhang, Z., Yang, S., & Zhao, Y. (2023). Classification of time-reversal-invariant crystals with gauge structures. Nature Communications, 14. https://doi.org/10.1038/s41467-023-36447-7
- Field, B., & Griffin, S. (2024). Symmetries of all lines in monolayer crystals.. Acta crystallographica. Section A, Foundations and advances. https://doi.org/10.1107/s205327332500422x
- Yan, Z. (2024). On Euclidean, spherical and hyperbolic crystallography. Theoretical and Natural Science. https://doi.org/10.54254/2753-8818/31/20241107
- Gratias, D., & Quiquandon, M. (2023). Crystallography of homophase twisted bilayers: coincidence, union lattices and space groups. Acta Crystallographica. Section A, Foundations and Advances, 79, 301 – 317. https://doi.org/10.1107/s2053273323003662

Further reading

- Mamedov, S. (2024). The Aspects of Dimensionality in the Analysis of Raman Spectra of 2D Materials. ECS Meeting Abstracts. https://doi.org/10.1149/ma2024-01121009mtgabs
- Landsberg, M., & Hankamer, B. (2007). Symmetry: A guide to its application in 2D electron crystallography.. Journal of structural biology, 160 3, 332-43. https://doi.org/10.1016/j.jsb.2007.07.002
- Moeck, P. (2018). Towards Generalized Noise-Level Dependent Crystallographic Symmetry Classifications of More or Less Periodic Crystal Patterns. Symmetry, 10, 133. https://doi.org/10.3390/sym10050133
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