

## Survey of Materials. Lecture 2

# Atomistic structure

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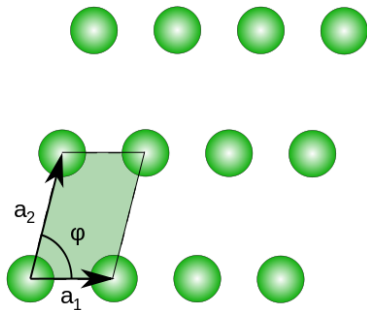
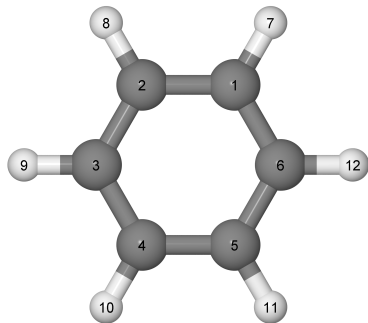
*October 28, 2018*

### *Outline*

- Why symmetry is important
- 2D crystallography
- 3D crystallography
- Nonperiodic solids
- Structure characterization and determination

## 2D crystallography

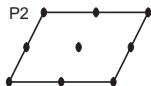
Space group = point group + translation symmetry



- Determine all 2D point groups
- Determine all 2D Bravais lattices

# 2D crystallography

2D space groups (17), point groups, Bravais lattices, and crystal systems (4)

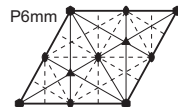
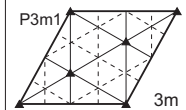
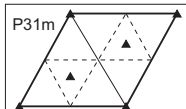
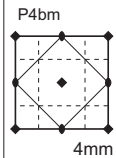
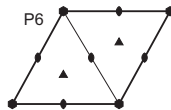
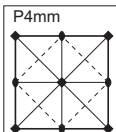
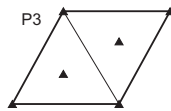
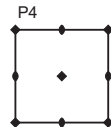
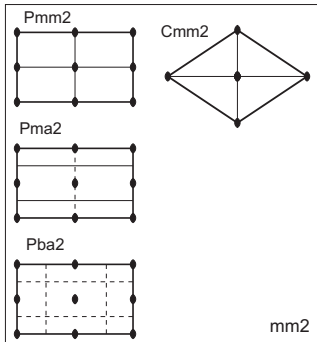
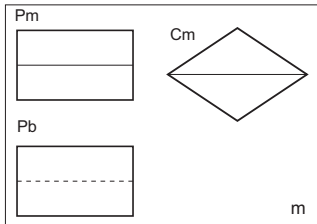


Bravais lattices:  
 P2 oblique  
 Pmm2 rectangular  
 Cmm2 rhombic  
 P4mm square  
 P6mm hexagonal

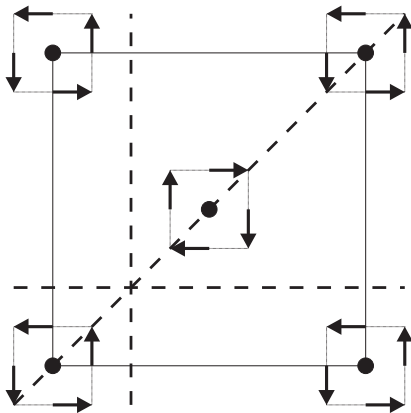
Point groups:

1-6  $C_{1-6}$   
 m  $D_1$   
 mm2  $D_2$   
 3m  $D_3$   
 4mm  $D_4$   
 6mm  $D_6$

Symmetries:

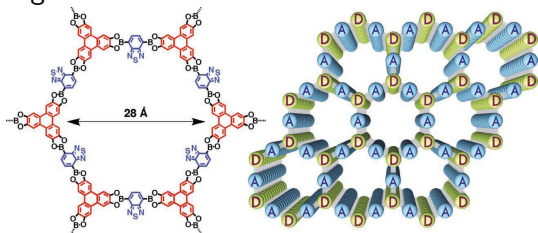


## 2D glide plane

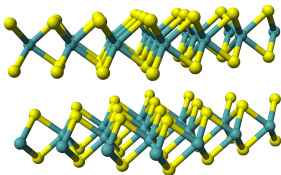


## 2D materials

- graphene, BN
- organic networks

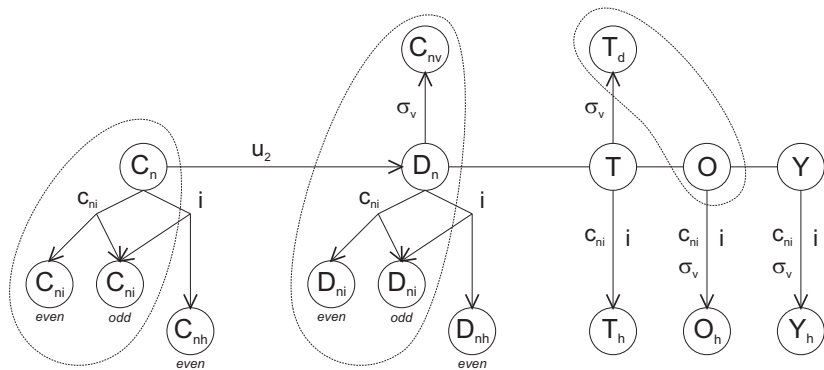


- MoS<sub>2</sub>



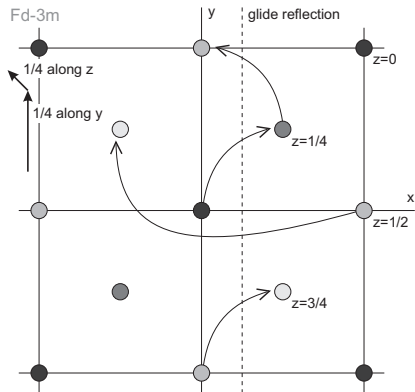
- P, As

# 3D point groups



# 3D symmetry elements

Axes								Planes	
	n	-n	$n_1$	$n_2$	$n_3$	$n_4$	$n_5$		
1	o							m	_____
2	●	●	●					a,b	-----
3	▲	▲	▲	▲				c	.....
4	◆	◆	◆	◆	◆			n	-----
6	●	●	●	●	●	●	●	d	----->

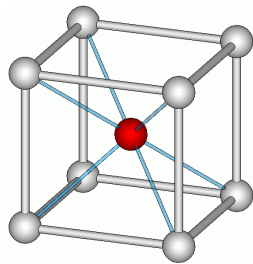
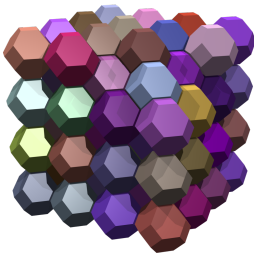
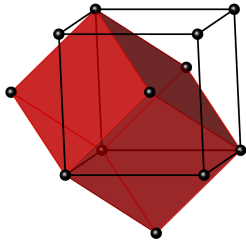


# 3D crystallography

Lecture of Artem Abakumov or any textbook



# Unit cell



	min.size	parallelepiped	symmetric
primitive	+	+	-
Wigner-Seitz	+	-	+
Bravais	-	+	+

# Classification of space groups

structural type	A4 (dia)	A3 (hcp)	A7 ( $\alpha$ -As)
space group	Fd-3m	P63/mmc	R-3m
arithmetic crystal class	Fm-3m	P6/mmm	R-3m
lattice centering	F	P	R
crystal class	m-3m	6/mmm	-3m
crystal family	c	h	h*

\* Lattice system is rhombohedral, crystal system is trigonal

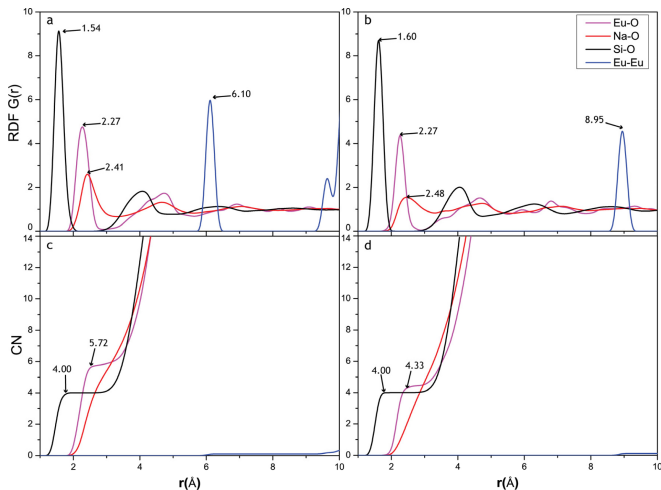
## Lattice system vs crystal system, crystal family

	space groups	lattice system	crystal family	crystal system
P1	... P-1	anorthic*	a	anorthic
P2	... C2/c	monoclinic	m	monoclinic
P222	... Imma	orthorhombic	o	orthorhombic
P4	... I4 <sub>1</sub> /acd	tetragonal	t	tetragonal
R3	... R-3c	rhombohedral	<b>h</b>	trigonal
P3	... P-3c1	<b>hexagonal</b>	<b>h</b>	<b>trigonal</b>
P6	... P6 <sub>3</sub> /mmc	hexagonal	<b>h</b>	hexagonal
P23	... Ia-3d	cubic	c	cubic

\* anorthic is also called triclinic

# Structure factor and radial distribution function

$$S(\mathbf{q}) = \frac{1}{N} \left| \sum_i e^{-i\mathbf{q}\mathbf{r}_i} \right| \equiv 1 + \rho \int_V e^{-i\mathbf{q}\mathbf{r}} g(\mathbf{r}) dV, \quad g(\mathbf{r}) = \sum_{i \neq 0} \delta(\mathbf{r} - \mathbf{r}_i)$$



# Summary and Resources

See summary [here](#)

- Wikipedia
- Bilbao Crystallographic Server
- Crystal structures
- References: [crystallography](#), [symmetry](#)
- [Textbooks](#) (sections General, Crystallography, Symmetry)

Visualization software:

- [Jmol](#)
- [Mercury](#)
- [Surface explorer](#) (online tool)