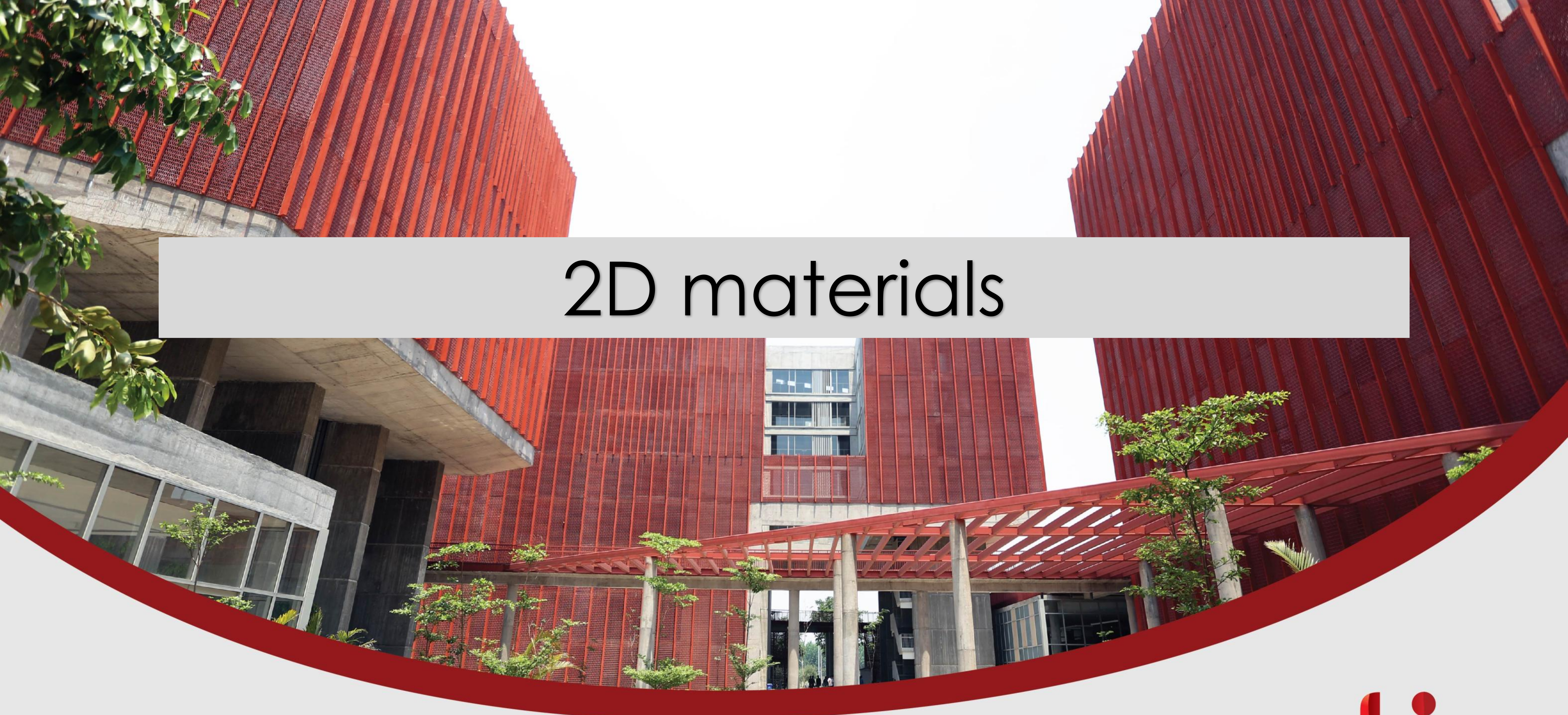

2D materials

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Syllabus

2D Materials and Graphene

- Structure, properties, and significance of graphene in electronic and thermal applications.
- Exploration of other 2D materials, such as transition metal dichalcogenides (TMDs) and their emerging applications.
- Applications of 2D materials in fields like sensors, quantum computing, and renewable energy.

From bulk to nanomaterials

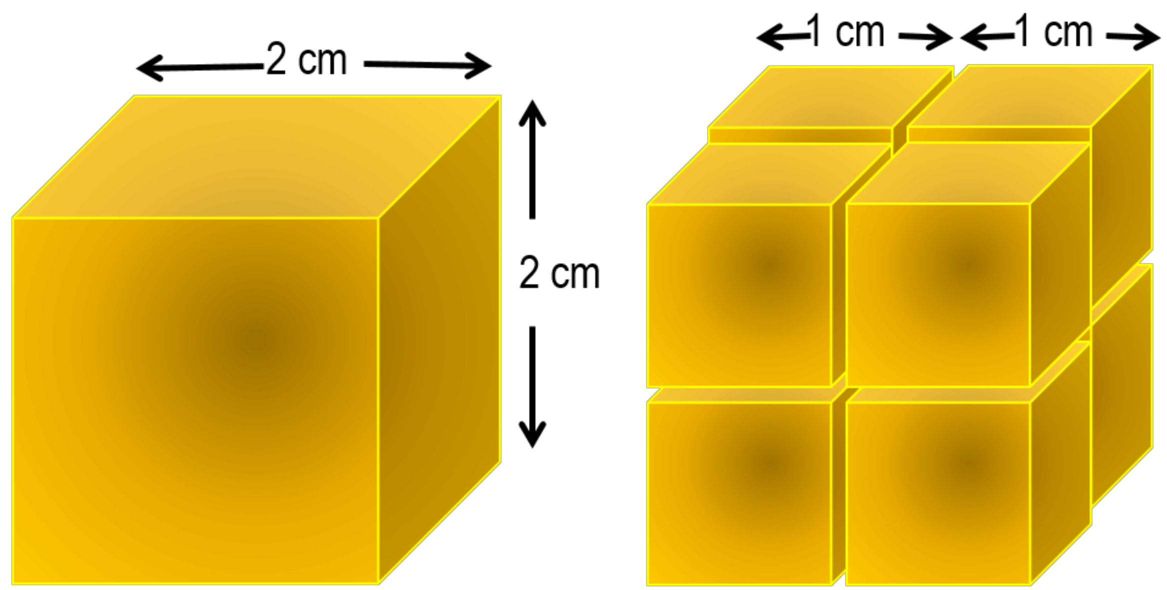
- Nanomaterials are a class of materials having sizes in the range of 1 to 100 nm.
- The term "nano" comes from the Greek prefix to "dwarf", or something very small (10^{-9} as the multiply factor)
- The concept of nanotechnology was only introduced in 1959 by Richard Feynman.
- Who proposed the idea of constructing molecular-level small machines

Richard Feynman

From bulk to nanomaterials

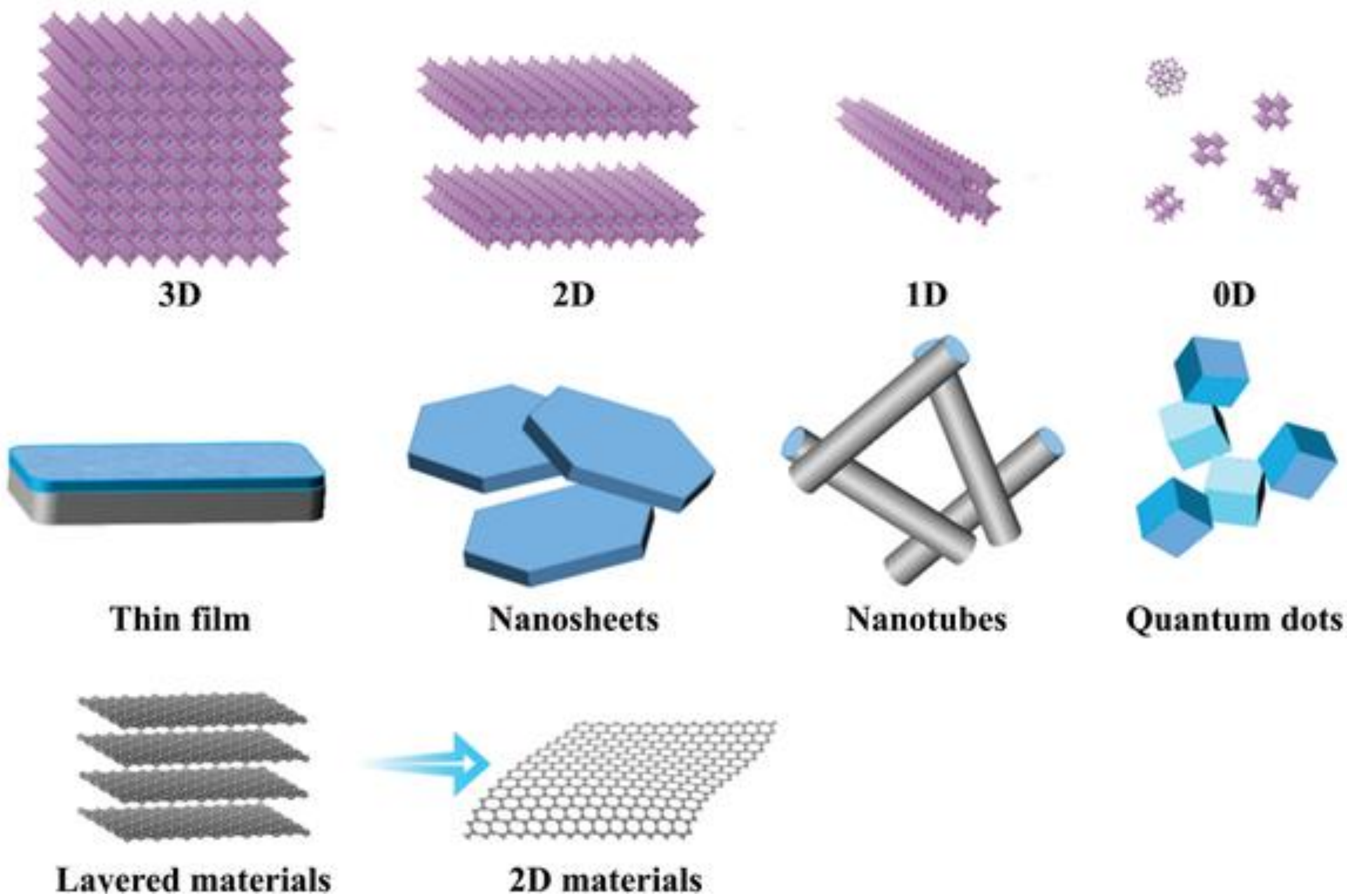
- Nanomaterials are either engineered or naturally occurring materials that have at least one dimension measuring between 1 and 100 nanometers (nm).

- Due to their extremely high surface area to volume ratio and quantum effects, nanomaterials exhibit unique properties that are not observed in larger-scale materials.



# of Cube (s)	Dimensions (cm)	Surface Area (l x l x 6 cm^2)	Volume (l x l x l cm^3)	Surface Area/Volume ratio
1	2 x 2	(2 x 2 x 6) = 24	(2 x 2 x 2) = 8	3
8	1 x 1	8 (1 x 1 x 6) = 48	8 (1 x 1 x 1) = 8	6

From bulk to nanomaterials



Quantum confinement & Dimension

Quantum confinement

In how many dimensions is it confined:

Quantum dots (0D): confined in all 3 dimensions

Nanotubes (1D): confined in 2 dimensions

Nanolayers (2D): confined in 1 dimension

Dimensions of nanomaterials

0D nanomaterials: confined to nanoscales in all dimensions. E.g. quantum dots

1D nanomaterials: 1 dimension is outside the nanoscale. E.g., nanotubes, nanowires, nanorods

2D nanomaterials: 2 dimensions are outside the nanoscale

3D nanomaterials: not confined to the nanoscale in any dimension. E.g., dispersion of nanoparticles, multi-nanolayers, etc.

Allotropes of Carbon

Allotropy or allotropism is the property of some chemical elements to exist in two or more different forms.

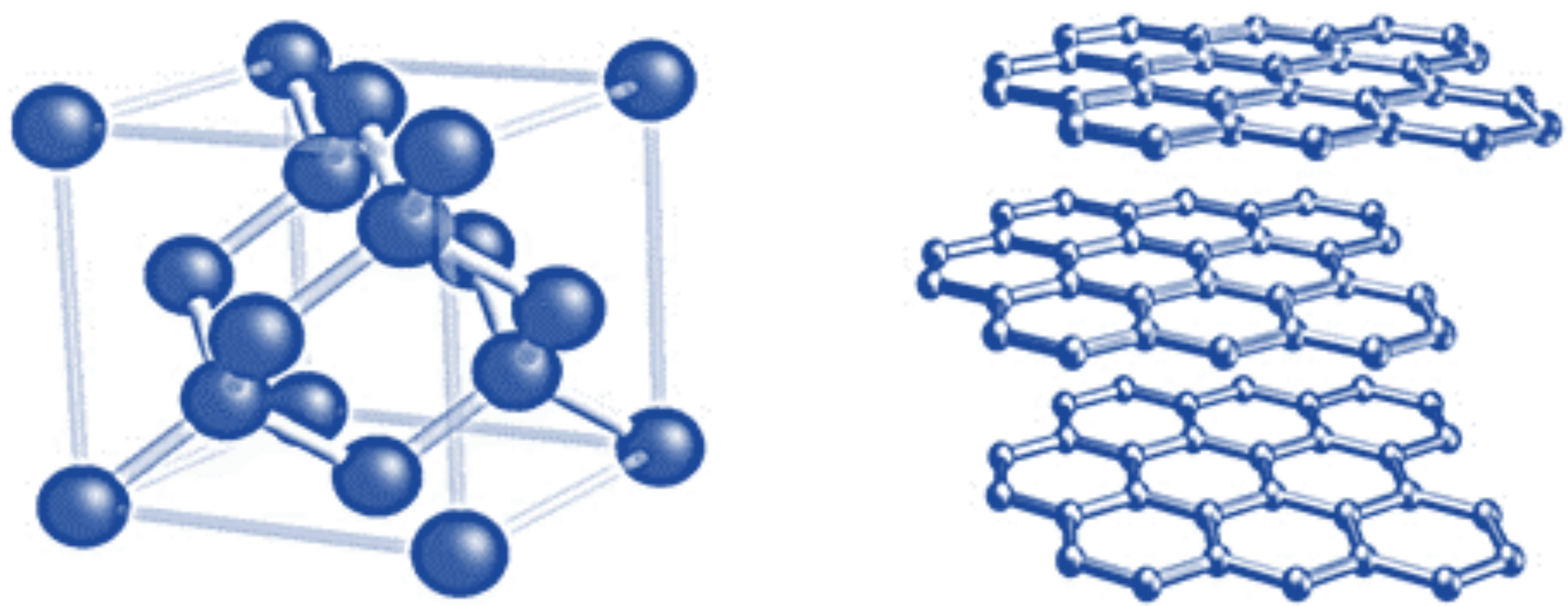
Why is diamond an insulator while graphite is a conductor?

Allotropes of Carbon

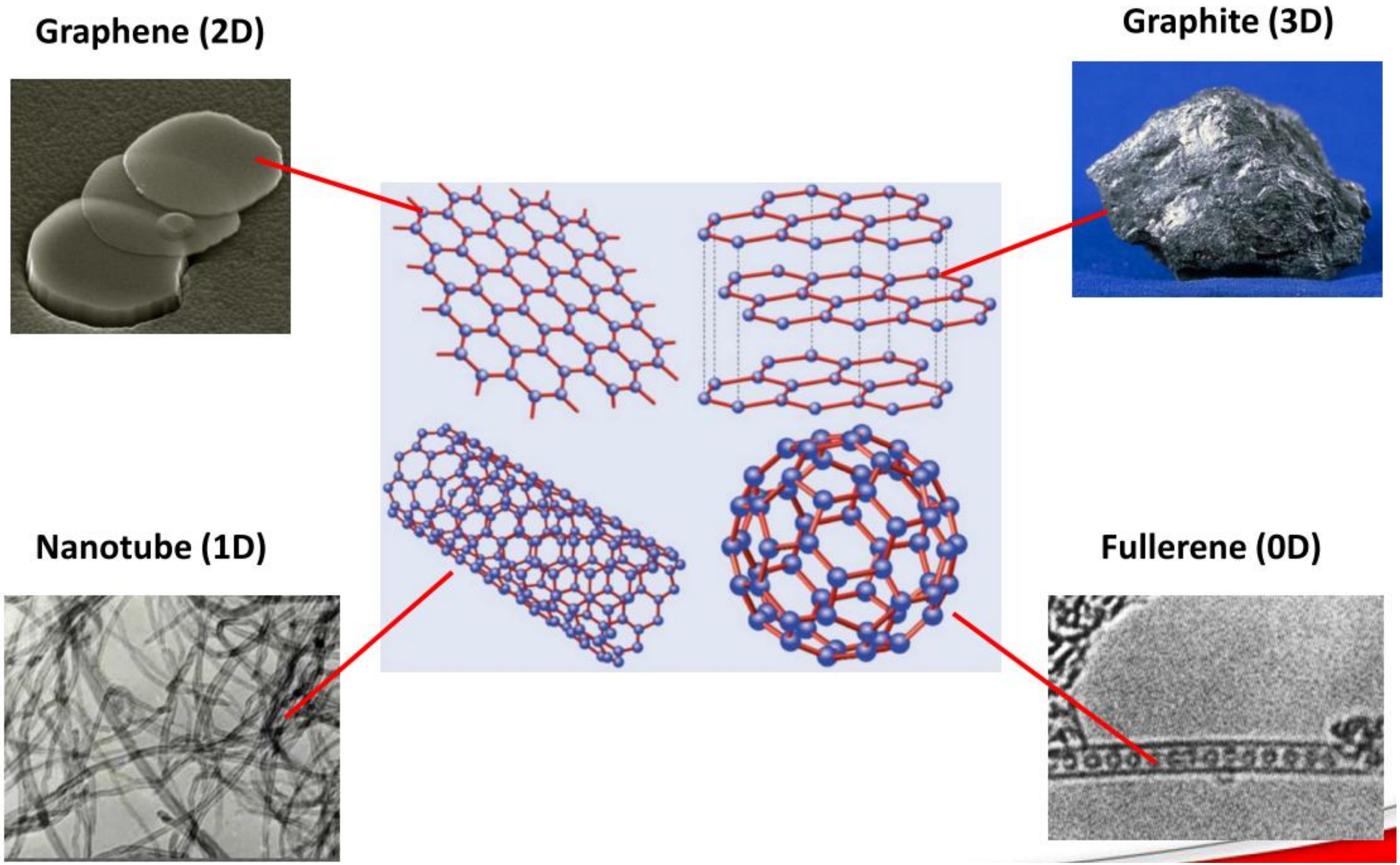
Diamond does not have free electrons.

Graphite has free electrons due to hybridization.

(a) Diamond (sp^3) (b) Graphite (sp^2)



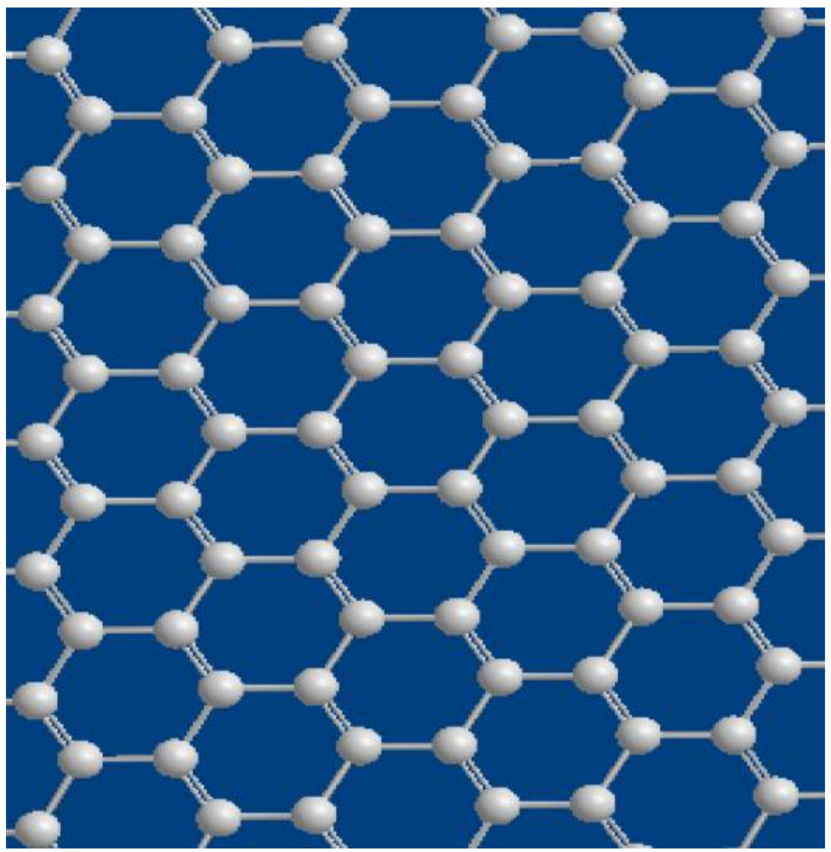
Carbon in all dimensionalities



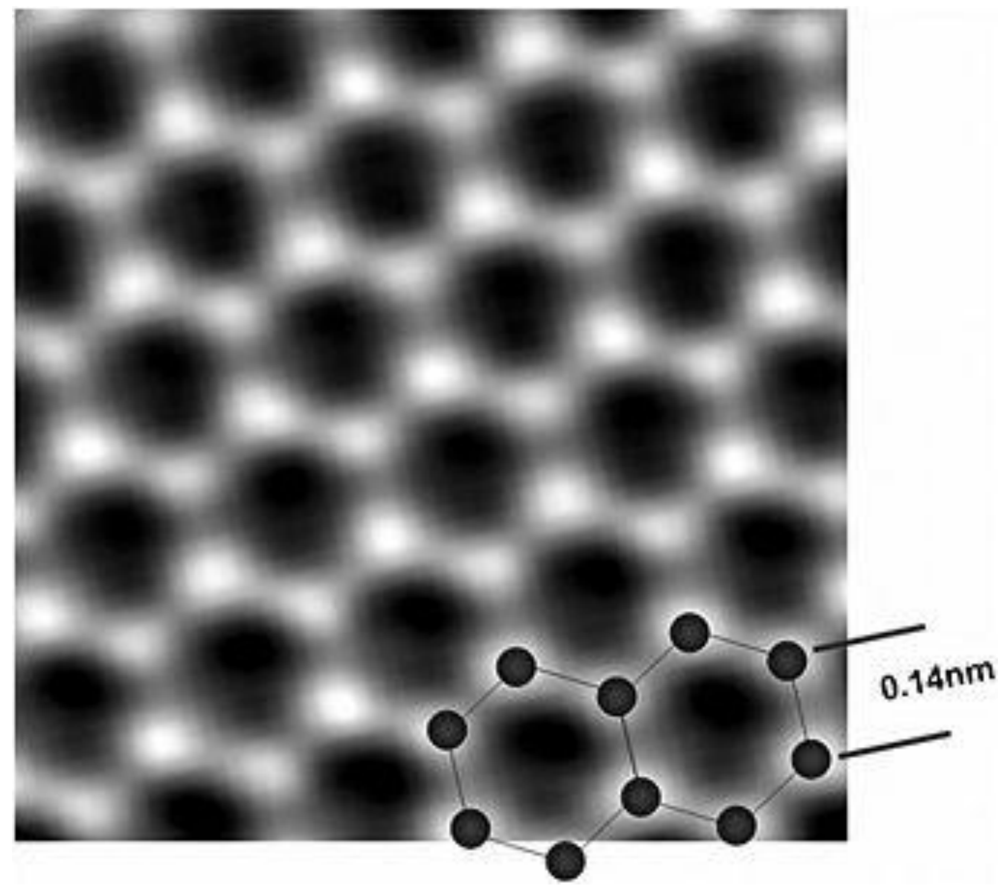
Graphene

Graphene *is a one-atom-thick planar sheet of sp²-bonded carbon atoms that are densely packed in a honeycomb crystal lattice*

The name 'graphene' comes from graphite + -ene = graphene

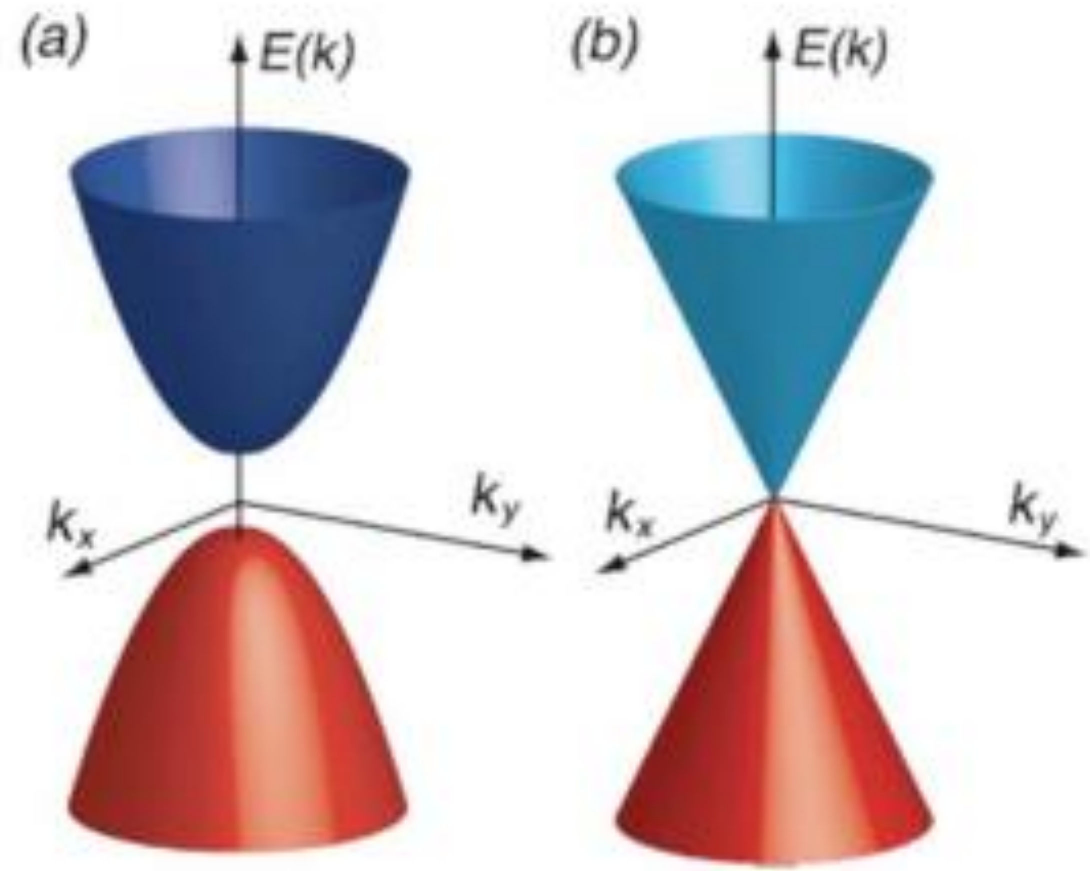


Molecular structure of graphene



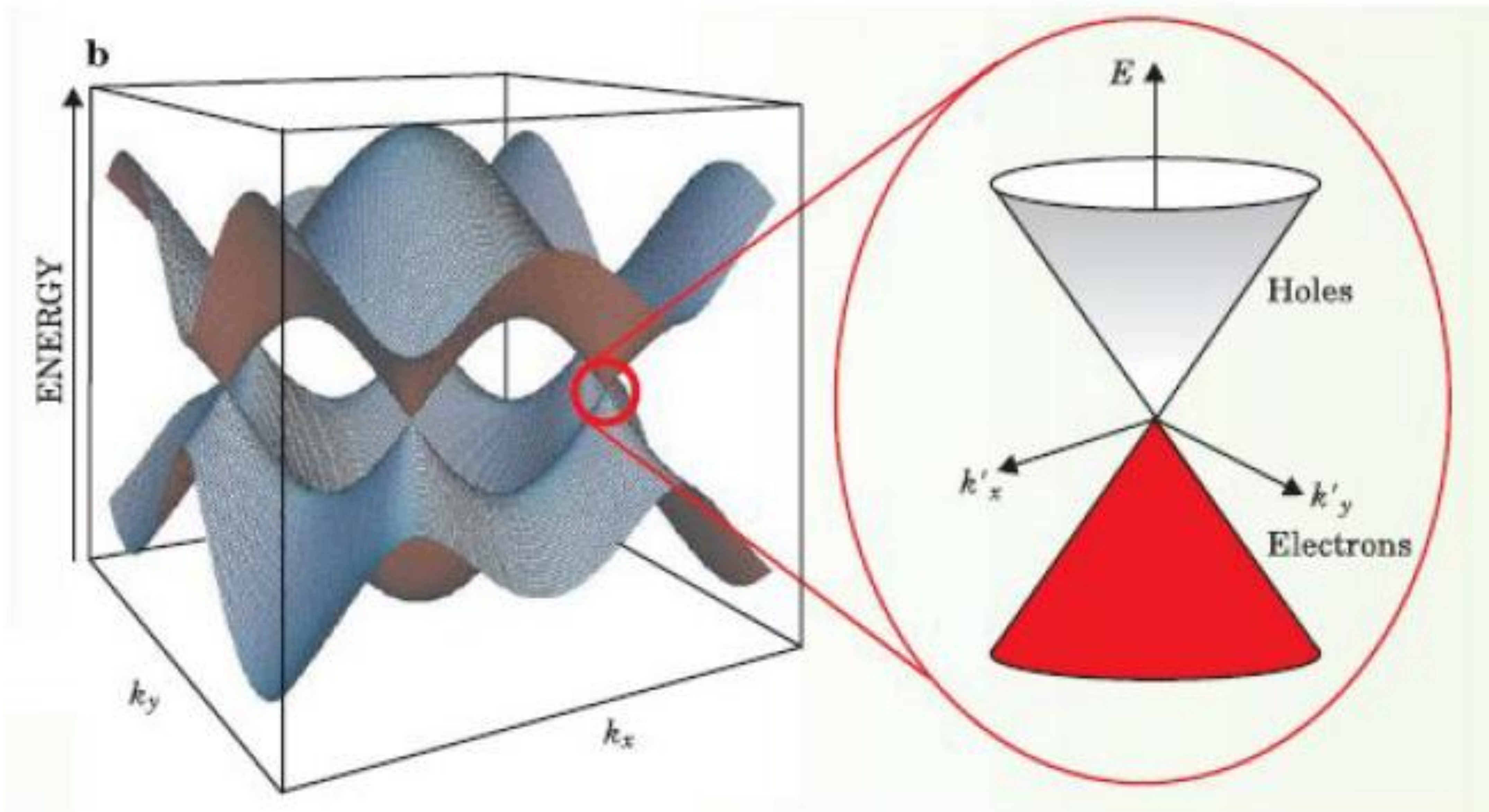
High-resolution transmission electron microscope images (TEM) of graphene

Graphene band structure



Energy dispersion relation for (a) conventional semiconductor; (b) graphene

Graphene band structure



Graphene vs. bulk semiconductors

	Si	GaAs	$In_{.53}Ga_{.47}As$	InAs	InSb	Graphene
Electron mobility (cm^2/Vs) at $n = 10^{12}\ cm^{-2}$	600	4,600	7,800	20,000	30,000	25,000 (flake) ~3000 (Epieaxial) ~2000 (CVD)
Electron saturation velocity (10^7 cm/s)	1	1.2	0.8	3.5	5	8
Ballistic mean free path (nm)	28	80	106	194	226	400
Band-gap (eV)	1.12	1.42	0.72	0.36	0.18	0

Electron saturation velocity (v_{sat}) is the maximum drift velocity an electron can reach in a semiconductor when subjected to a strong electric field.

Ballistic mean free path (often called simply mean free path, λ) is the average distance an electron (or carrier) travels without scattering. When device dimensions are smaller than λ, electron transport becomes ballistic rather than diffusive.

Electrical conductivity

Material	Electrical Conductivity ($S \cdot m^{-1}$)
Graphene	**~ 10^8**
Silver	63.0×10^6
Copper	59.6×10^6
Gold	45.2×10^6

Thermal conductivity

Material	**Thermal conductivity W/(m·K)**
Lead	35.3
Aluminium	237 (pure)
Gold	318
Copper	401
Silver	429
Graphene	**(4840±440) - (5300±480)**

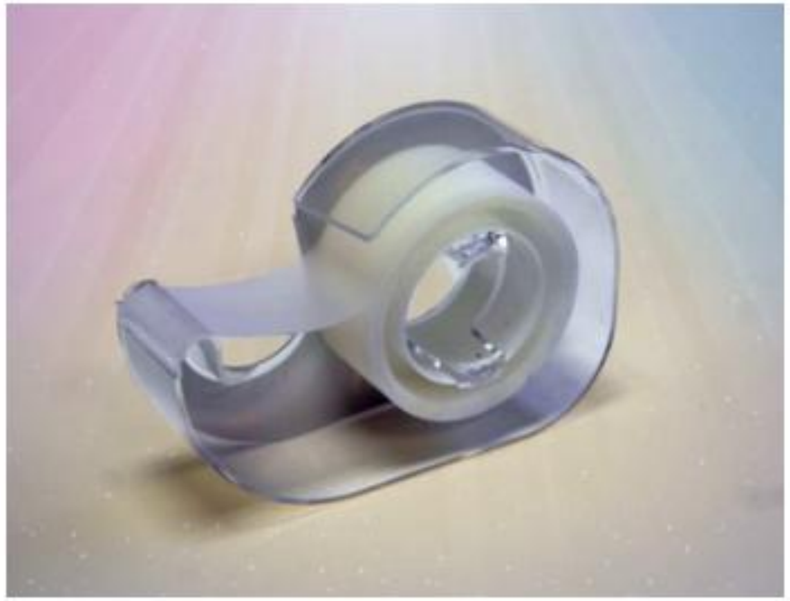
Mechanical Property

- High Young's modulus (~1,100 GPa)
- High fracture strength (125 GPa)
- Graphene is the strongest material ever measured; stronger than structural steel (210 GPa)

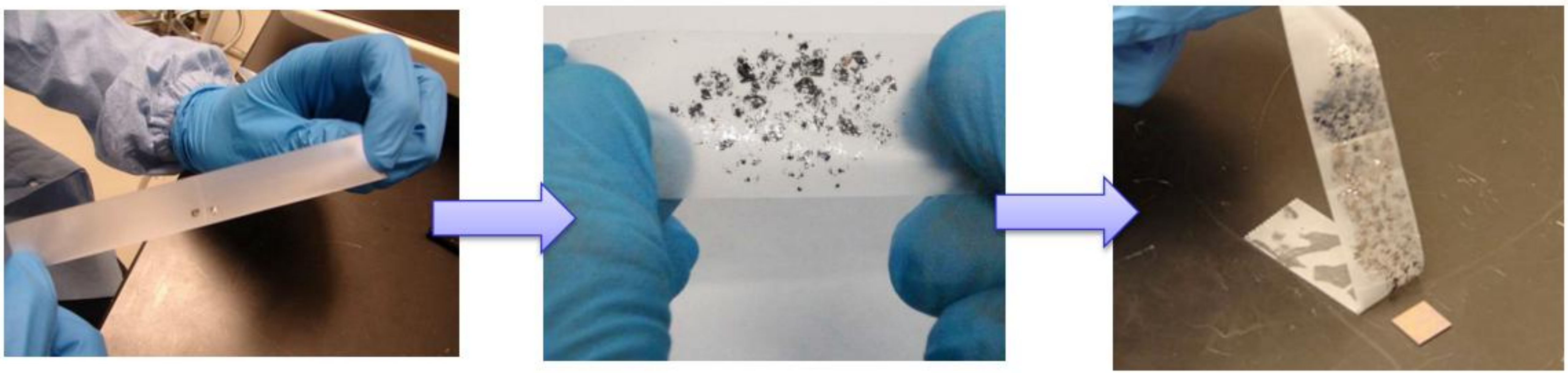
A representation of a diamond tip with a two-nanometer radius indenting into a single atomic sheet of graphene *(Science,* **321** (5887): 385)

How to make Graphene?

Or try this at home



You may win one of these ten years ago....



Also works for other 2D Materials!

Graphene preparation methods

Top-down approach (From graphite)

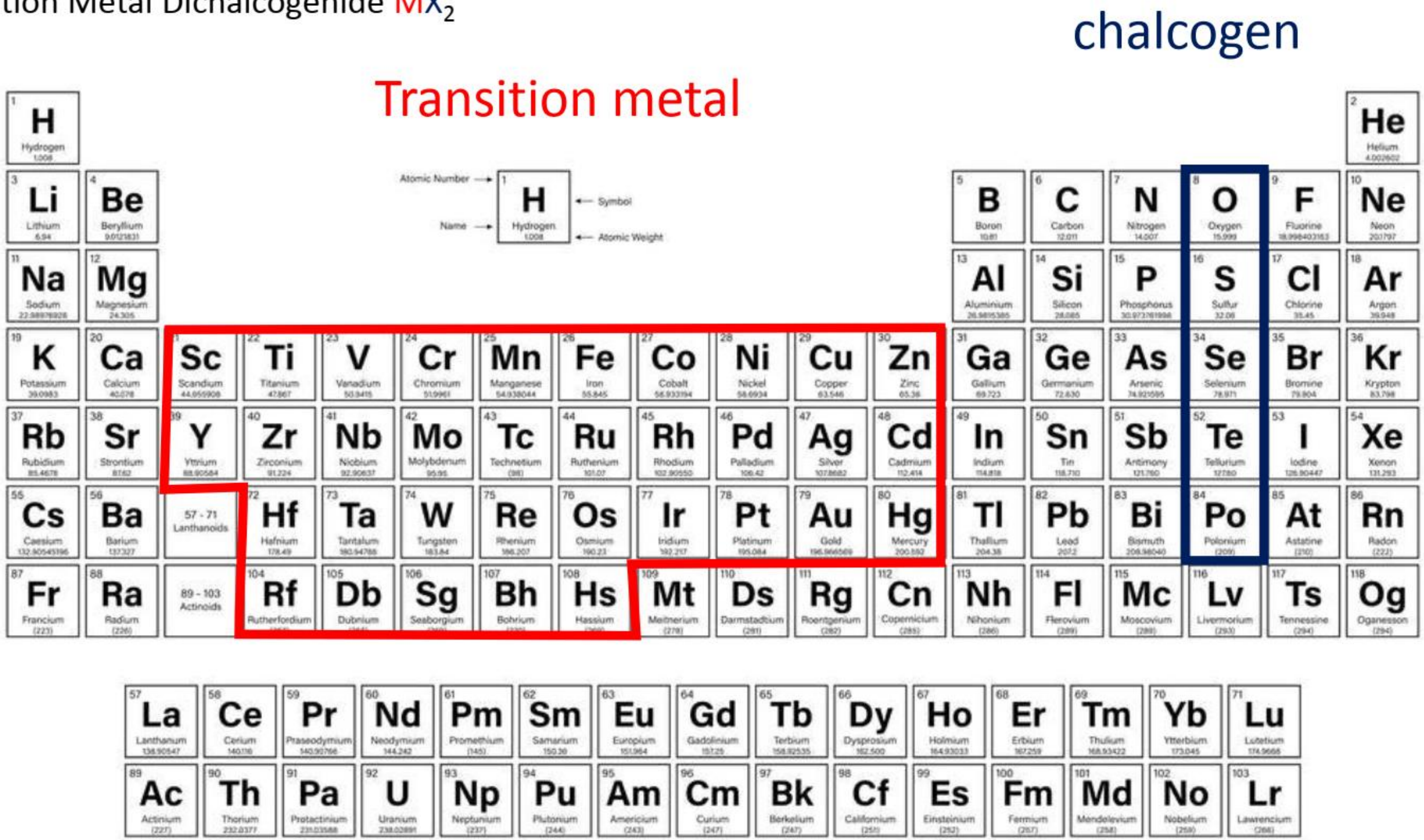
- Micromechanical exfoliation of graphite (Scotch tape or peel-off method)
- Creation of colloidal suspensions from graphite oxide or graphite intercalation compounds (GICs)

Bottom up approach (from carbon precursors)

- By chemical vapour deposition (CVD) of hydrocarbon
- By epitaxial growth on electrically insulating surfaces such as SiC
- Total Organic Synthesis

Beyond Graphene

Transition Metal Dichalcogenide MX_2

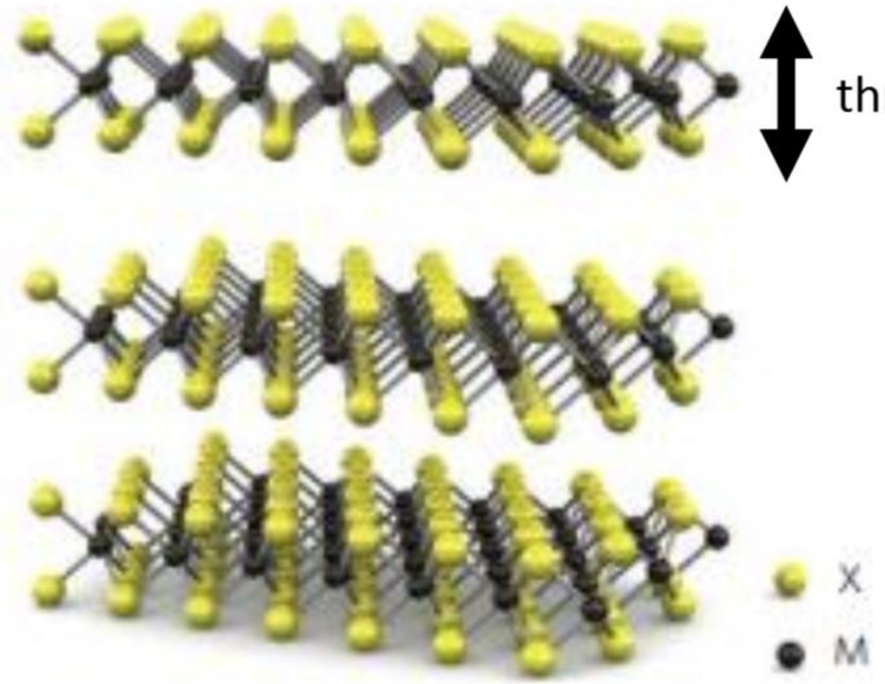


Example of TMD

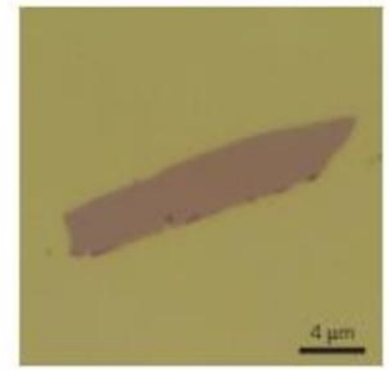
bulk crystal MoS_2

For lubrication

Ampere cop



crystal structure

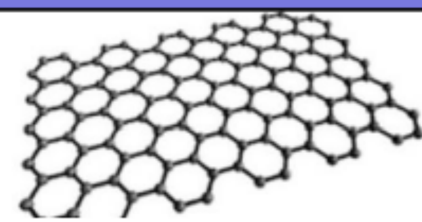
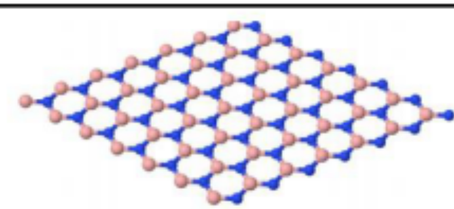
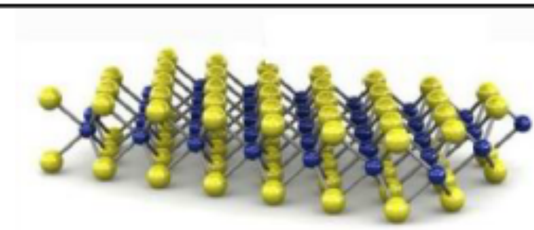
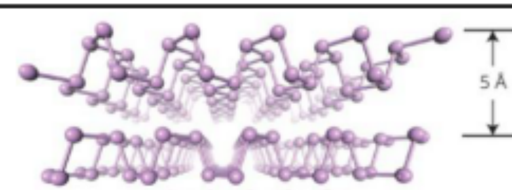


Optical microscopy image

Nat. Nanotechnol. **2012**, *7*, 699.

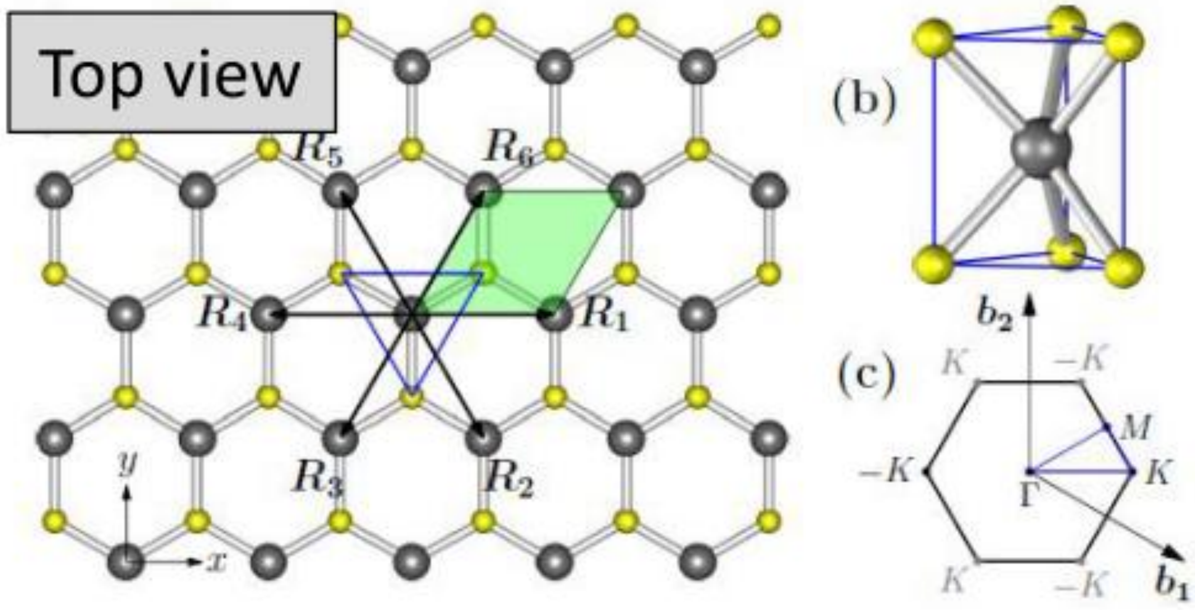
2-D materials

- More than 140 two-dimensional (2-D) materials, and the number is still growing
- Covering insulators, semiconductors, and metals

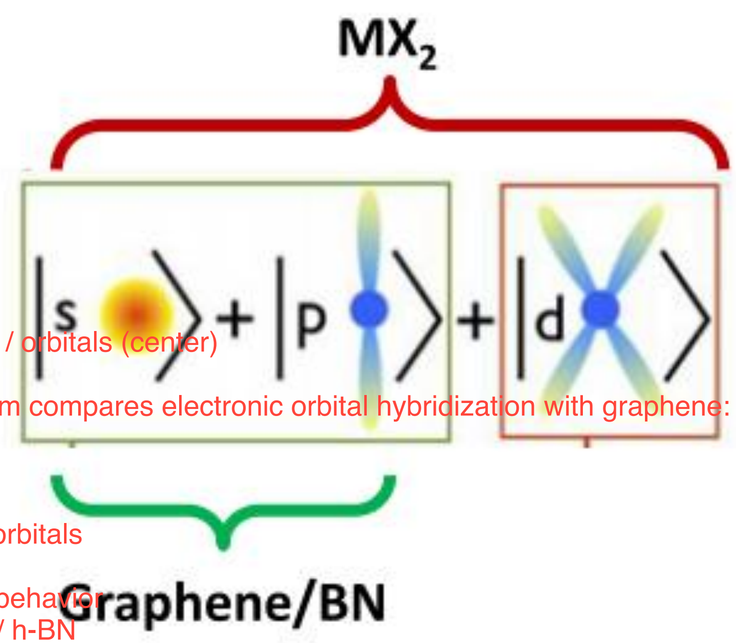
Material	Structure	Bandgap	Mobility (cm^2/Vs)
Graphene		0	1000-100,000
h-BN		~7.2 eV (indirect)	-
TMD (MX_2) M: W, Mo, Hf, Zr, Ti, Cr, Ta X: S, Se, Te		0.6 – 2.3 eV, and depending on layer #	10~500
Black Phosphorus (BP)		~2 eV (Monolayer) ~0.3eV (few layer)	100~1000

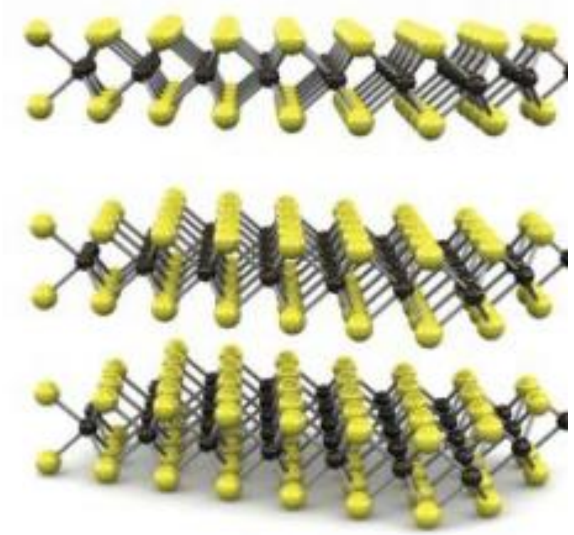
2-D Transition Metal Dichalcogenide

- Lattice structure (1H)



M = Transition metal (Mo, W, etc.)
X = Chalcogen (S, Se, Te)





4. Bonding / orbitals (center)

The diagram compares electronic orbital hybridization with graphene:

Material

Dominant orbitals

Electronic behavior
Graphene / h-BN

s + p orbitals

Light, massless electron behavior
MX_2 (TMDs)

d orbitals (from M) + p orbitals (from X)

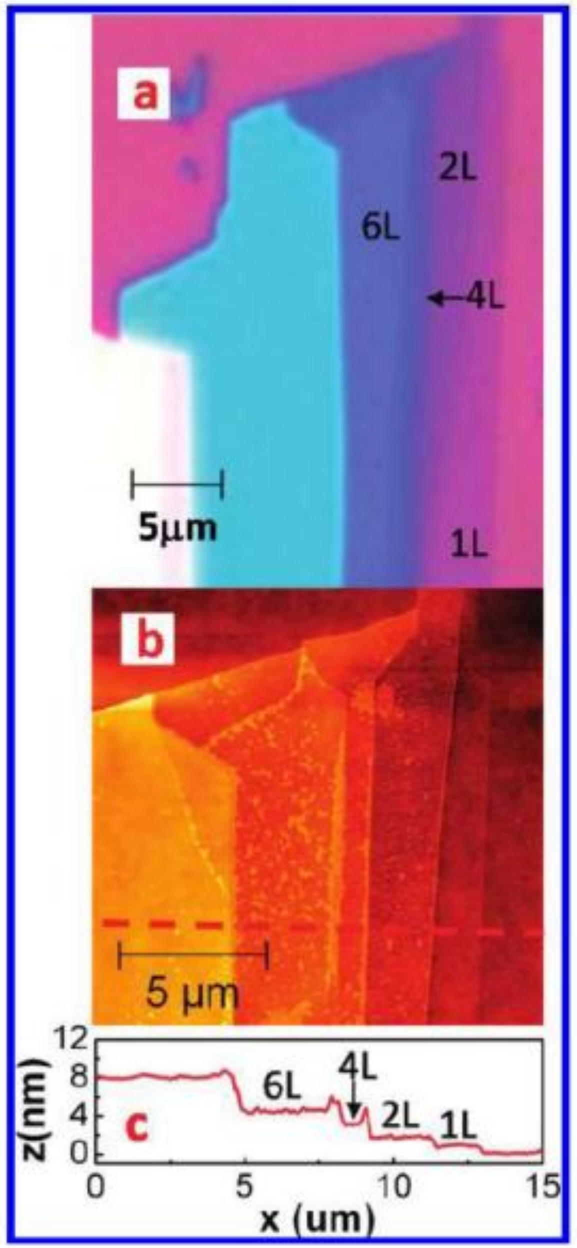
Strong spin–orbit coupling, direct bandgap, valley splitting

Because of the involvement of d orbitals, electrons in TMDs:

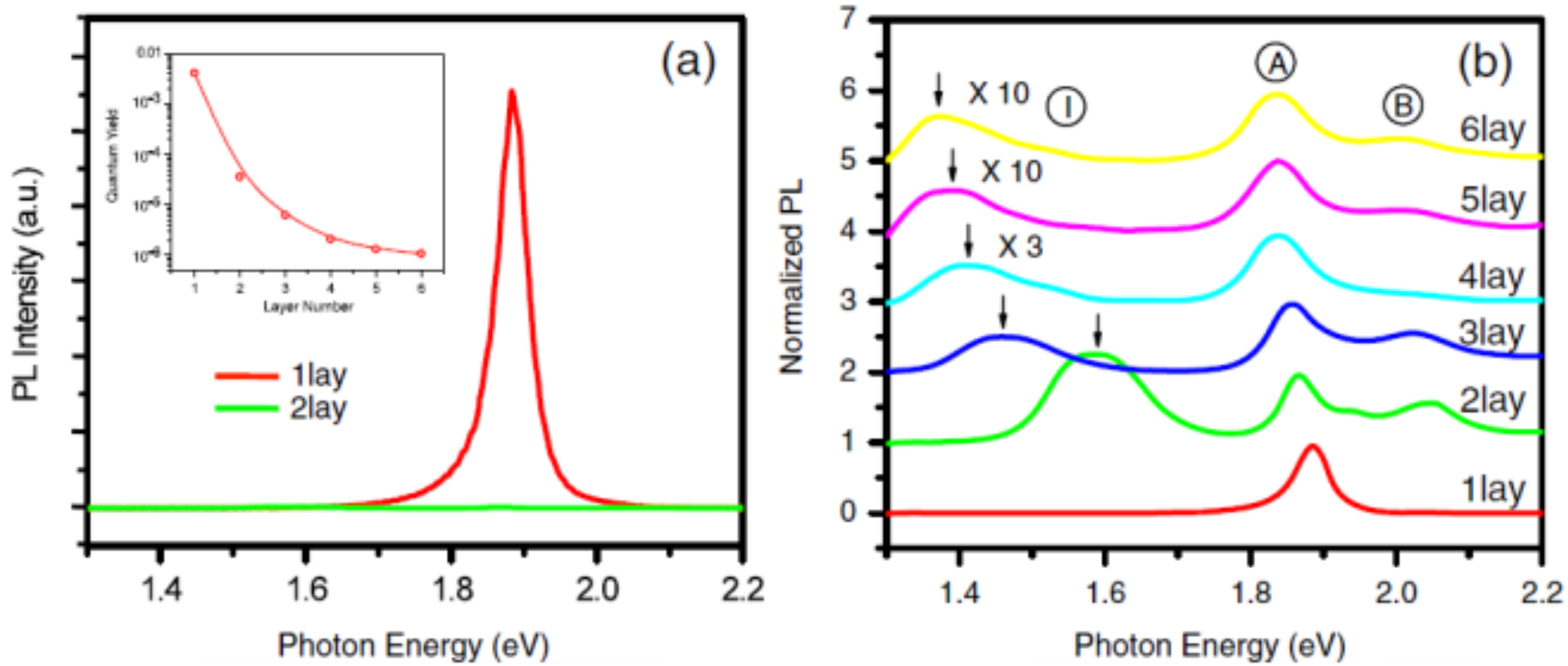
Have a bandgap (unlike graphene)

Show spin–valley coupling and strong optical absorption

TMD direct and indirect band gap



10^4 times stronger photoluminescence (PL) in 1 layer MoS_2



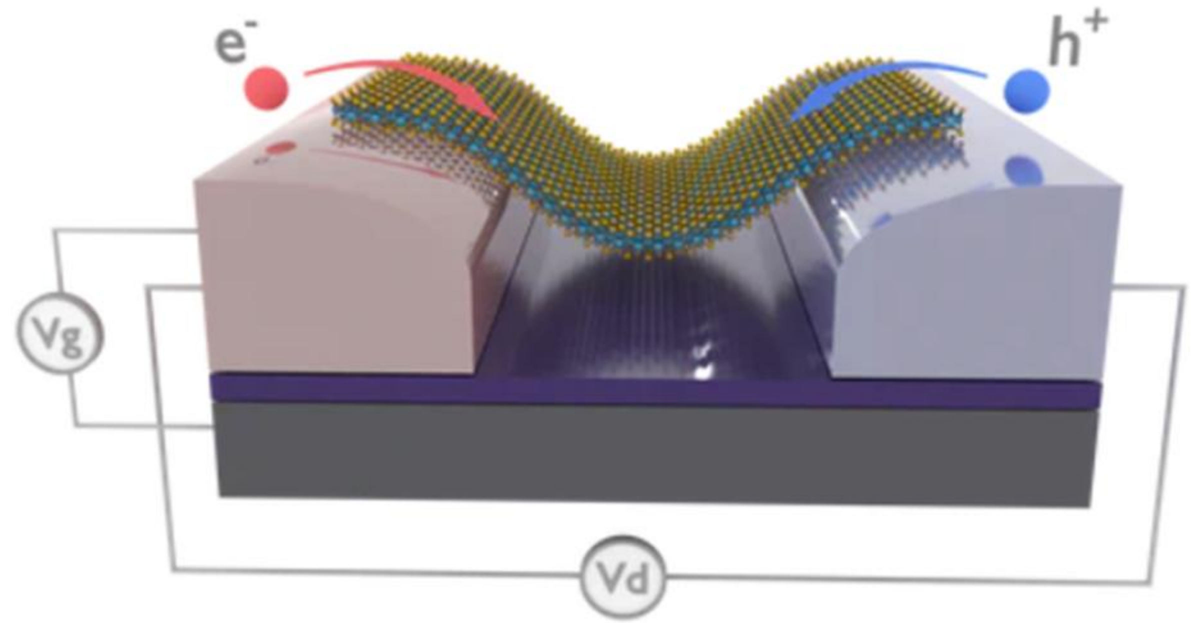
Applications

2-D materials have the potential to revolutionize many electronics applications such as solar cells, transistors, camera sensors, digital screens, and semiconductors.

Applications

Field-effect transistors (FETs) have been made from various semiconducting 2D materials, including transition metal dichalcogenides (TMDCs) and black phosphorus. Their high charge mobility and moderate band gaps make them strong candidates for this application.

A transistor formed from a monolayer of TMDC spanning metal electrodes



Graphene Field-Effect Transistor (FET)