



2D materials

Thapar Institute of Engineering & Technology
(Deemed to be University)
Bhadson Road, Patiala, Punjab, Pin-147004
Contact No. : +91-175-2393201
Email : info@thapar.edu

ti
THAPAR INSTITUTE
OF ENGINEERING & TECHNOLOGY
(Deemed to be University)

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

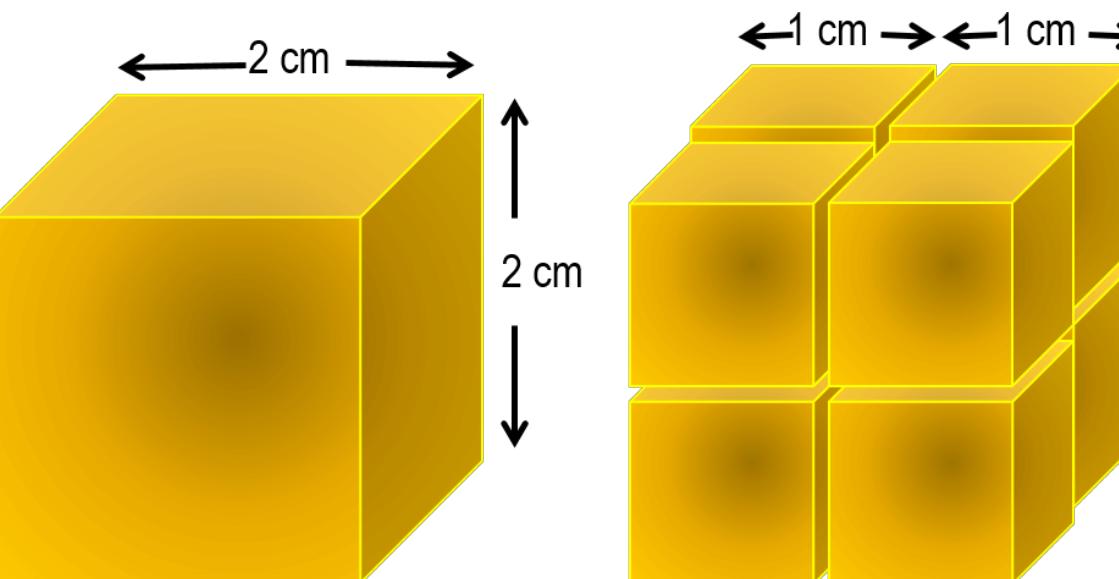
- Nanomaterials are a class of materials having sizes in the range of 1 to 100 nm.
- The term “nano” comes from the Greek prefix to “dwarf”, or something very small (10^{-9} as the multiply factor)
- The concept of nanotechnology was only introduced in 1959 by Richard Feynman.
- Who proposed the idea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



Richard Feynman

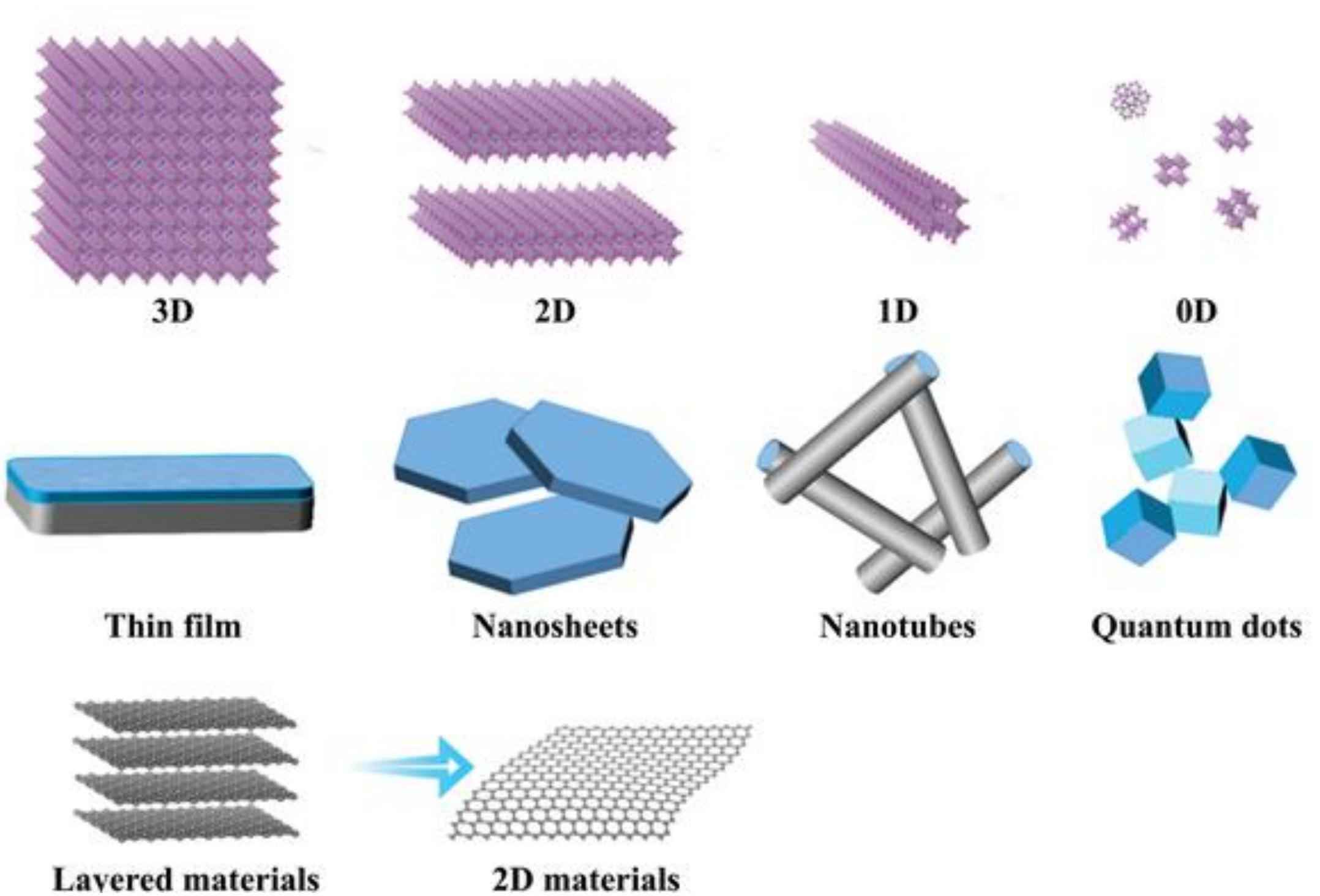
From bulk to nanomaterials

- 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 ($l \times l \times 6 \text{ cm}^2$)	Volume ($l \times l \times l \text{ cm}^3$)	Surface Area/Volume ratio
1	2 x 2	$(2 \times 2 \times 6) = 24$	$(2 \times 2 \times 2) = 8$	3
8	1 x 1	$8 (1 \times 1 \times 6) = 48$	$8 (1 \times 1 \times 1) = 8$	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

7

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



Diamond



Graphite



Fullerene

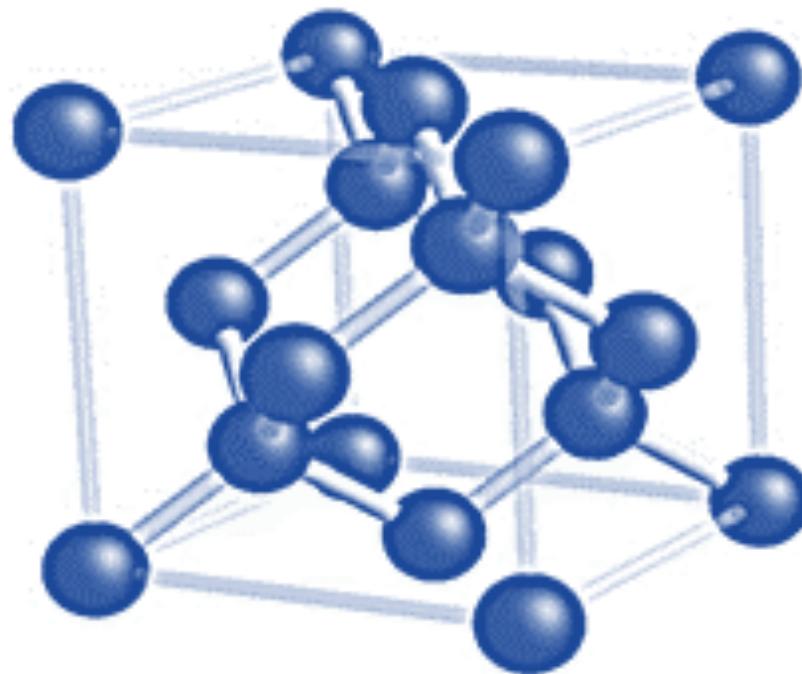
Why is diamond an insulator while graphite is a conductor?

Allotropes of Carbon

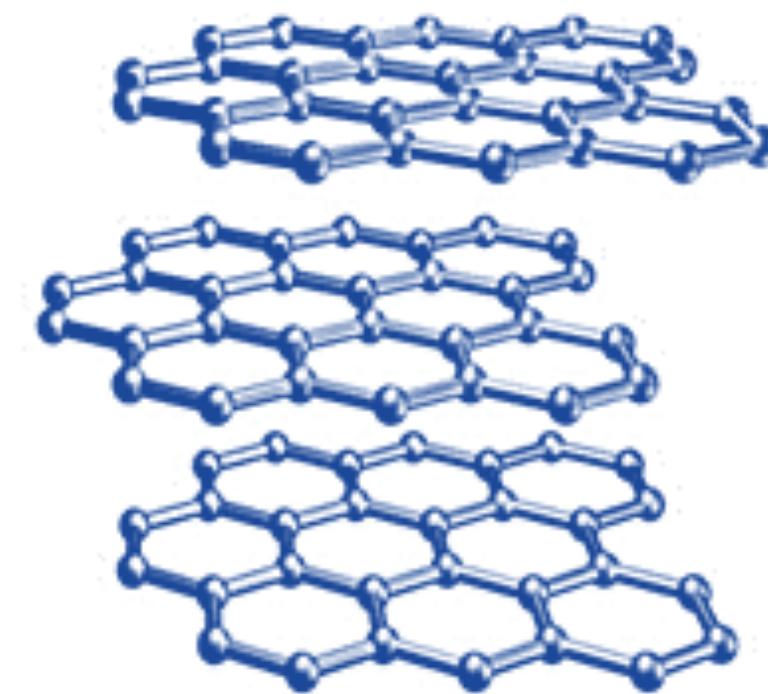
Diamond does not have free electrons.

Graphite has free electrons due to hybridization.

(a) Diamond (sp^3)

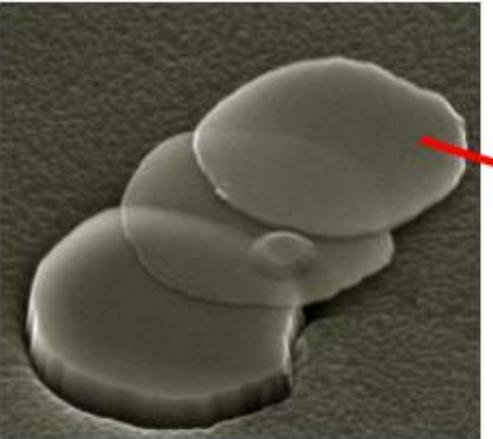


(b) Graphite (sp^2)



Carbon in all dimensionalities

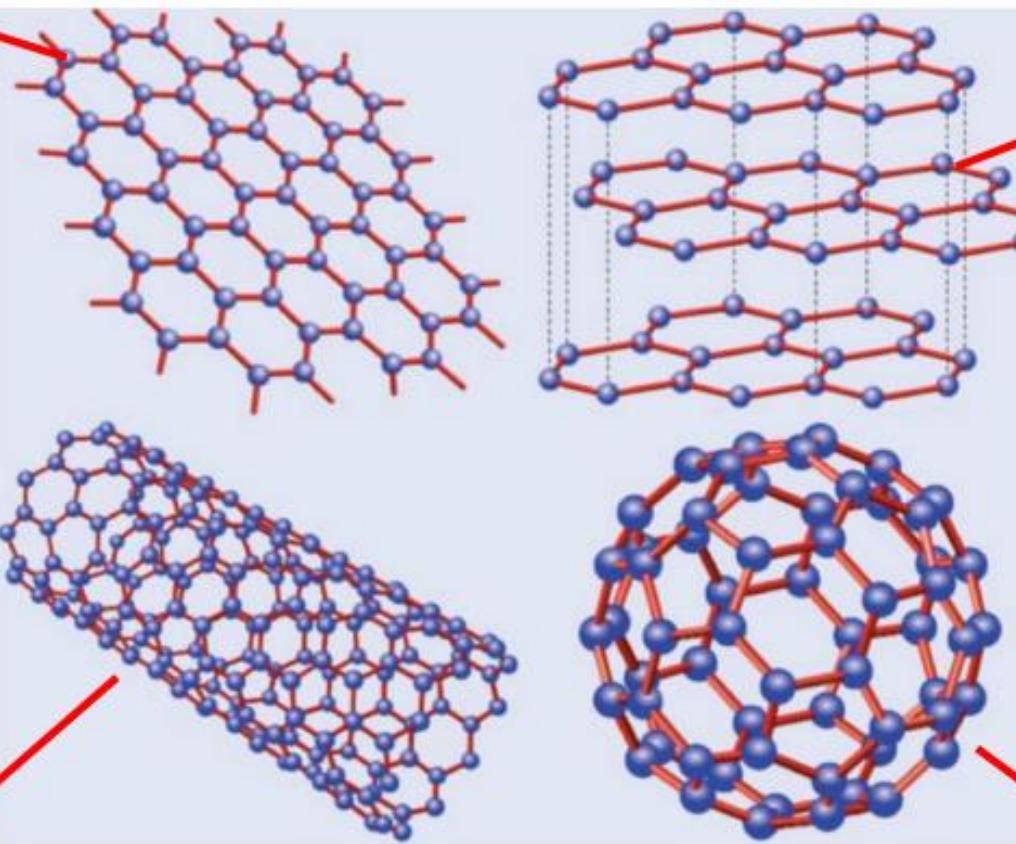
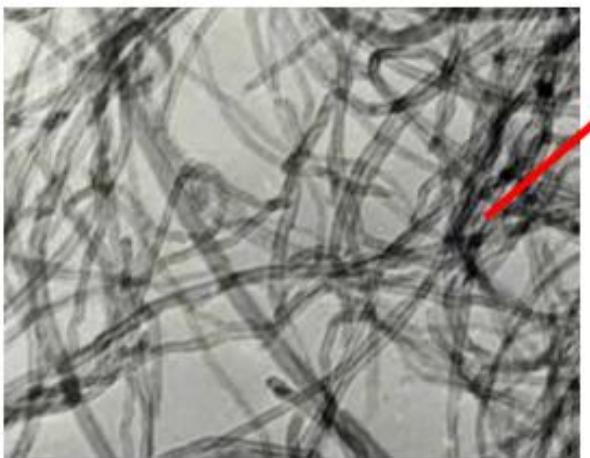
Graphene (2D)



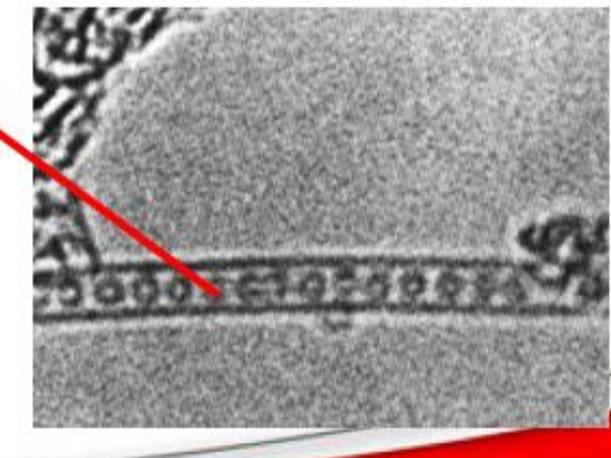
Graphite (3D)



Nanotube (1D)



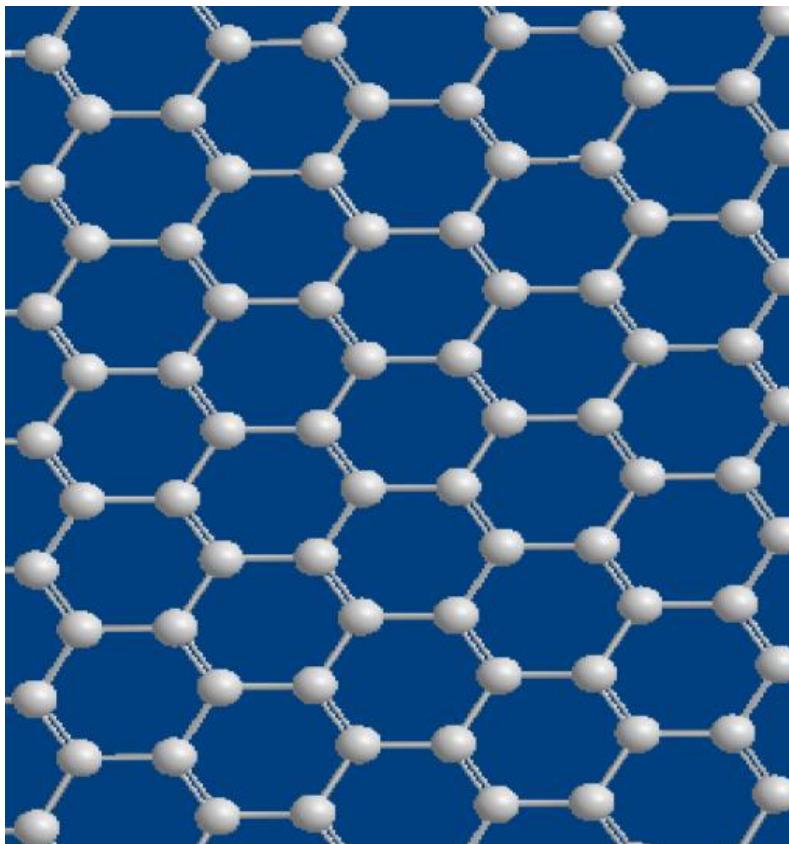
Fullerene (0D)



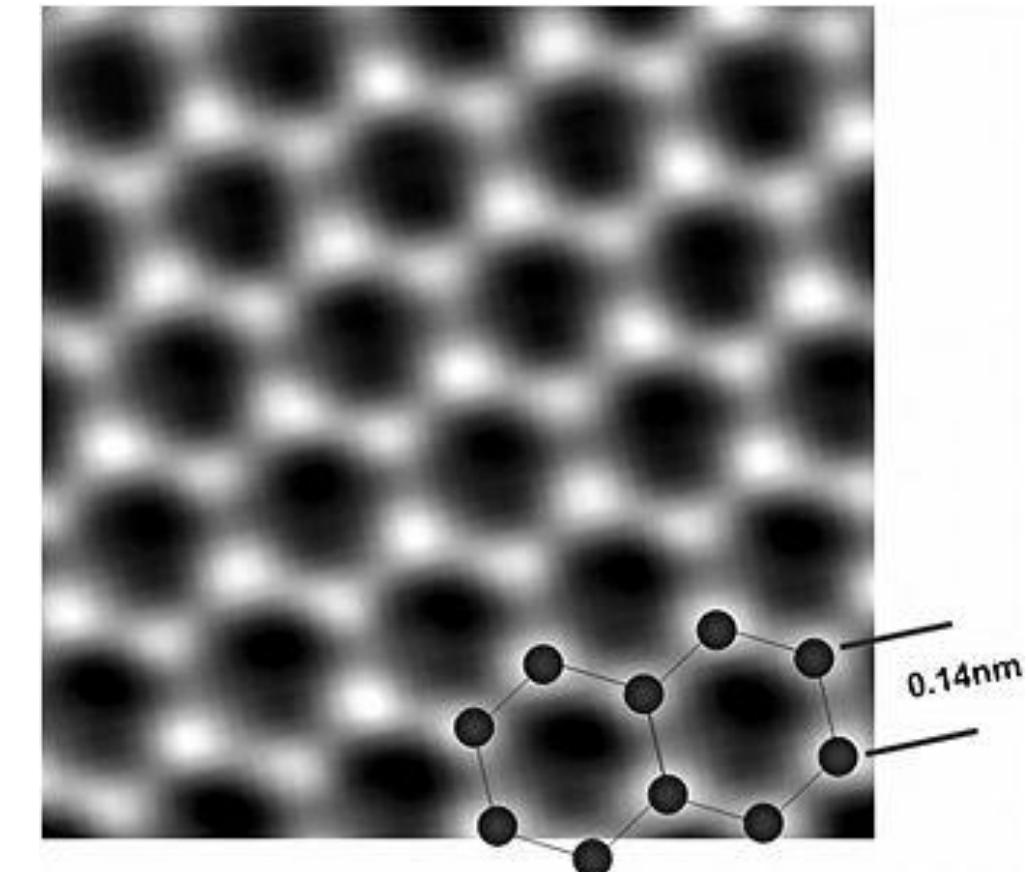
Graphene

Graphene is a one-atom-thick planar sheet of sp^2 -bonded carbon atoms that are densely packed in a honeycomb crystal lattice

The name ‘graphene’ comes from graphite + -ene = **graphene**

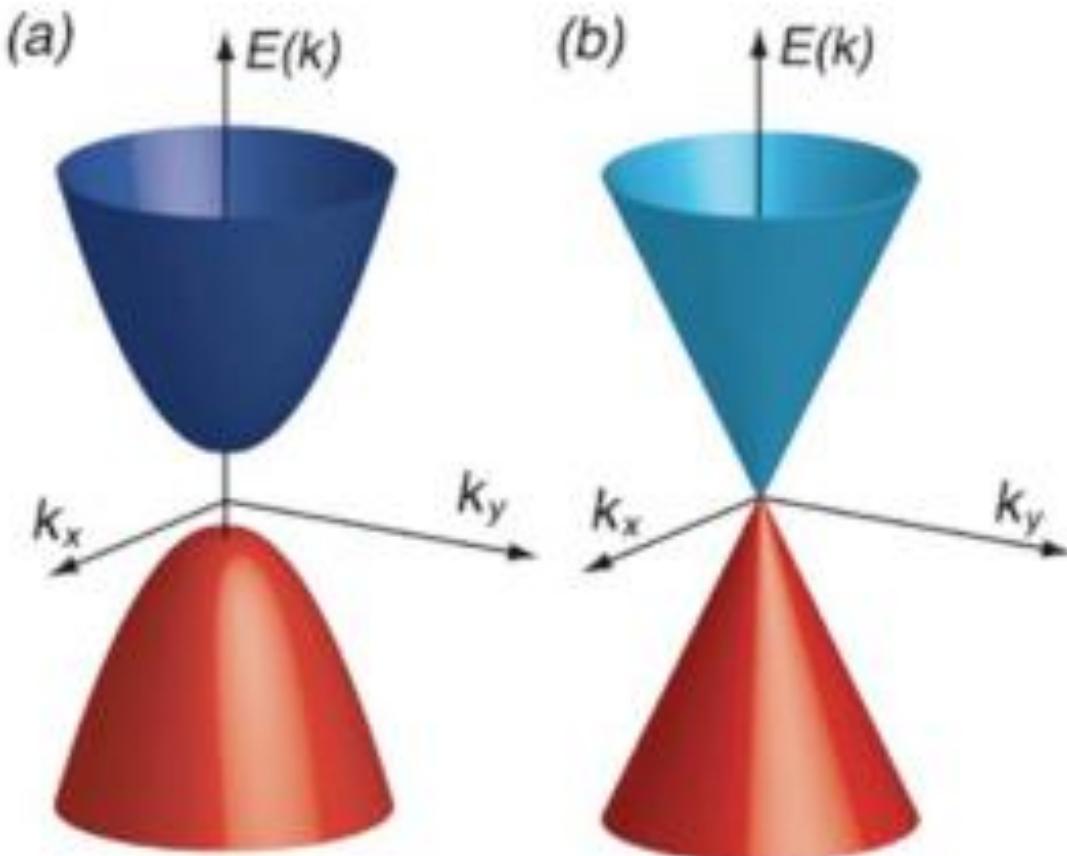


Molecular structure of graphene



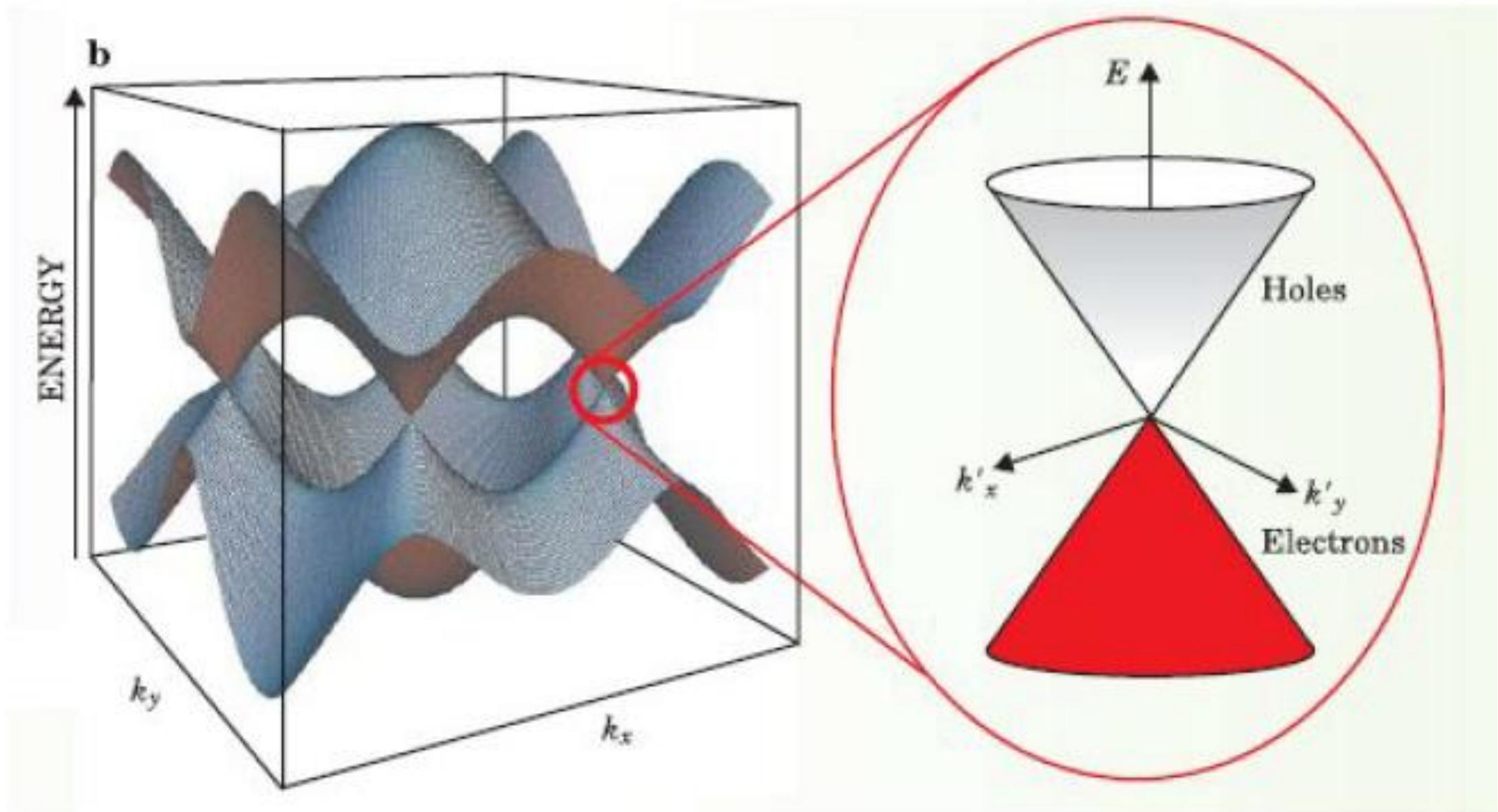
High-resolution transmission electron microscope images (TEM) of graphene

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 (Epiaxial) ~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 ($\text{S} \cdot \text{m}^{-1}$)
Graphene	$\sim 10^8$
Silver	63.0×10^6
Copper	59.6×10^6
Gold	45.2×10^6

Thermal conductivity

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

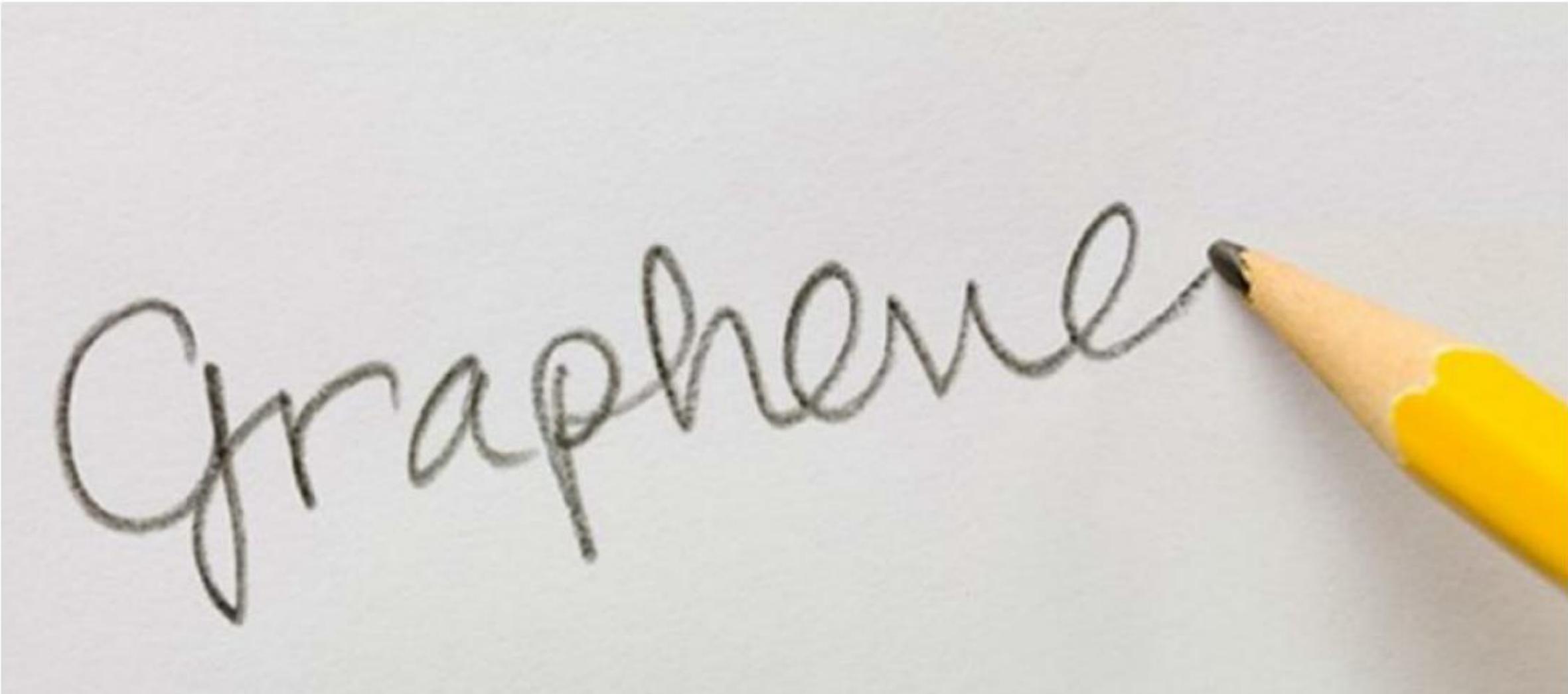
Mechanical Property

- 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)

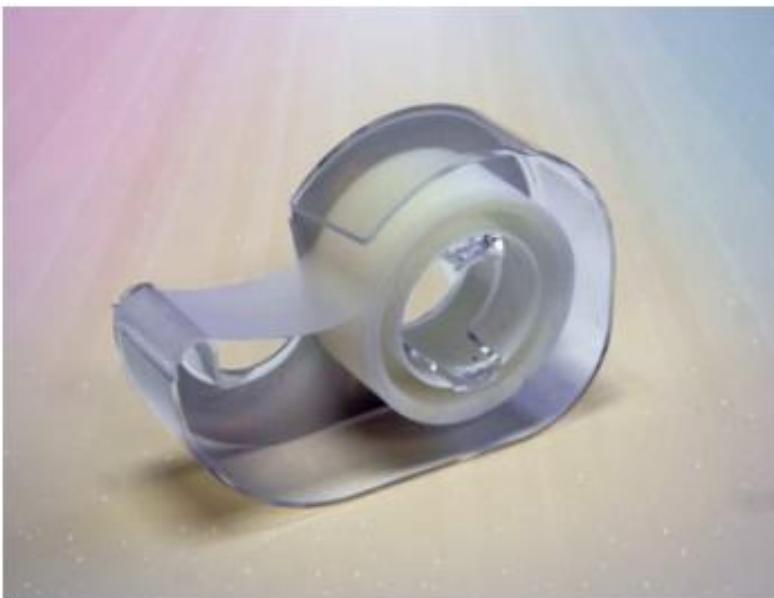


A representation of a diamond tip with a two-nanometer radius indenting into a single atomic sheet of graphene (*Science*, 321 (5887): 385)

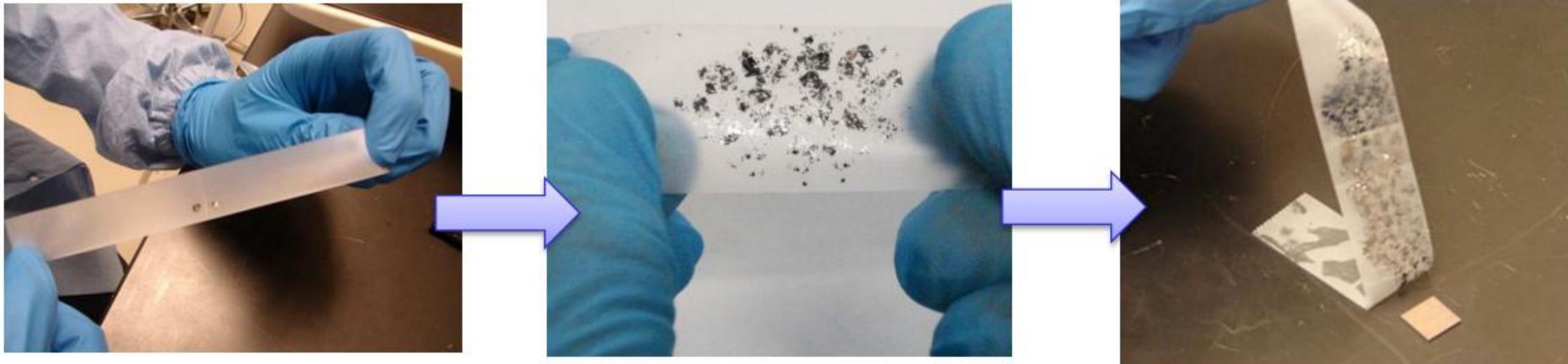
How to make Graphene?



Or try this at home



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



Also works for other 2D Materials!

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

Transition Metal Dichalcogenide MX_2

chalcogen

Transition metal

The periodic table is shown with several elements highlighted:

- Transition metals:** A red box highlights the first 20 transition metals: Scandium (Sc) through Hafnium (Hf), plus Rutherfordium (Rf), Dubnium (Db), Seaborgium (Sg), Bohrium (Bh), Hassium (Hs), and Meitnerium (Mt).
- Chalcogens:** A blue box highlights the second-period chalcogens: Oxygen (O), Sulfur (S), and Selenium (Se).
- Lanthanoids:** A red box highlights the Lanthanoid series from Lanthanum (La) to Lutetium (Lu).
- Actinoids:** A red box highlights the Actinoid series from Actinium (Ac) to Lawrencium (Lr).

1 H Hydrogen 1.008	2 He Helium 4.002602																
3 Li Lithium 6.94	4 Be Beryllium 9.01283	5 B Boron 10.8	6 C Carbon 12.011	7 N Nitrogen 14.007	8 O Oxygen 15.999	9 F Fluorine 18.998403183	10 Ne Neon 20.1797										
11 Na Sodium 22.98979828	12 Mg Magnesium 24.305	13 Al Aluminum 26.98153865	14 Si Silicon 28.085	15 P Phosphorus 30.973761998	16 S Sulfur 32.06	17 Cl Chlorine 35.45	18 Ar Argon 39.948										
19 K Potassium 39.0983	20 Ca Calcium 40.078	21 Sc Scandium 44.95908	22 Ti Titanium 47.867	23 V Vanadium 50.9415	24 Cr Chromium 52.9991	25 Mn Manganese 54.938044	26 Fe Iron 55.845	27 Co Cobalt 58.93194	28 Ni Nickel 58.6934	29 Cu Copper 63.546	30 Zn Zinc 65.38	31 Ga Gallium 69.723	32 Ge Germanium 72.630	33 As Arsenic 74.92165	34 Se Selenium 78.917	35 Br Bromine 79.804	36 Kr Krypton 83.798
37 Rb Rubidium 85.4678	38 Sr Strontium 87.62	39 Y Yttrium 88.90584	40 Zr Zirconium 91.224	41 Nb Niobium 92.90637	42 Mo Molybdenum 95.95	43 Tc Technetium (98)	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.90550	46 Pd Palladium 106.42	47 Ag Silver 107.8662	48 Cd Cadmium 112.416	49 In Indium 113.418	50 Sn Tin 118.710	51 Sb Antimony 121.760	52 Te Tellurium 127.80	53 I Iodine 126.90447	54 Xe Xenon 131.293
55 Cs Caesium 132.90545196	56 Ba Barium 137.327	57 - 71 Lanthanoids	72 Hf Hafnium 178.49	73 Ta Tantalum 180.54785	74 W Tungsten 183.84	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.217	78 Pt Platinum 195.084	79 Au Gold 196.96768	80 Hg Mercury 200.597	81 Tl Thallium 204.38	82 Pb Lead 207.2	83 Bi Bismuth 208.986040	84 Po Polonium (209)	85 At Astatine (210)	86 Rn Radon (222)
87 Fr Francium (223)	88 Ra Radium (226)	89 - 103 Actinoids	104 Rf Rutherfordium (261)	105 Db Dubnium (262)	106 Sg Seaborgium (263)	107 Bh Bohrium (264)	108 Hs Hassium (265)	109 Mt Meitnerium (279)	110 Ds Darmstadtium (281)	111 Rg Röntgenium (282)	112 Cn Copernicium (285)	113 Nh Nhonium (286)	114 Fl Flerovium (289)	115 Mc Moscovium (289)	116 Lv Livermorium (293)	117 Ts Tennessine (294)	118 Og Oganesson (294)

57 La Lanthanum 138.90547	58 Ce Cerium 140.116	59 Pr Praseodymium 140.95766	60 Nd Neodymium 144.242	61 Pm Promethium 145	62 Sm Samarium 150.30	63 Eu Europium 151.964	64 Gd Gadolinium 157.25	65 Tb Terbium 158.92535	66 Dy Dysprosium 162.500	67 Ho Holmium 164.93033	68 Er Erbium 167.259	69 Tm Thulium 168.93422	70 Yb Ytterbium 173.045	71 Lu Lutetium 174.9666
89 Ac Actinium (227)	90 Th Thorium 232.0377	91 Pa Protactinium 231.03588	92 U Uranium 238.02891	93 Np Neptunium (237)	94 Pu Plutonium (244)	95 Am Americium (243)	96 Cm Curium (247)	97 Bk Berkelium (247)	98 Cf Californium (251)	99 Es Einsteinium (252)	100 Fm Fermium (257)	101 Md Mendelevium (258)	102 No Nobelium (258)	103 Lr Lawrencium (261)

Example of TMD

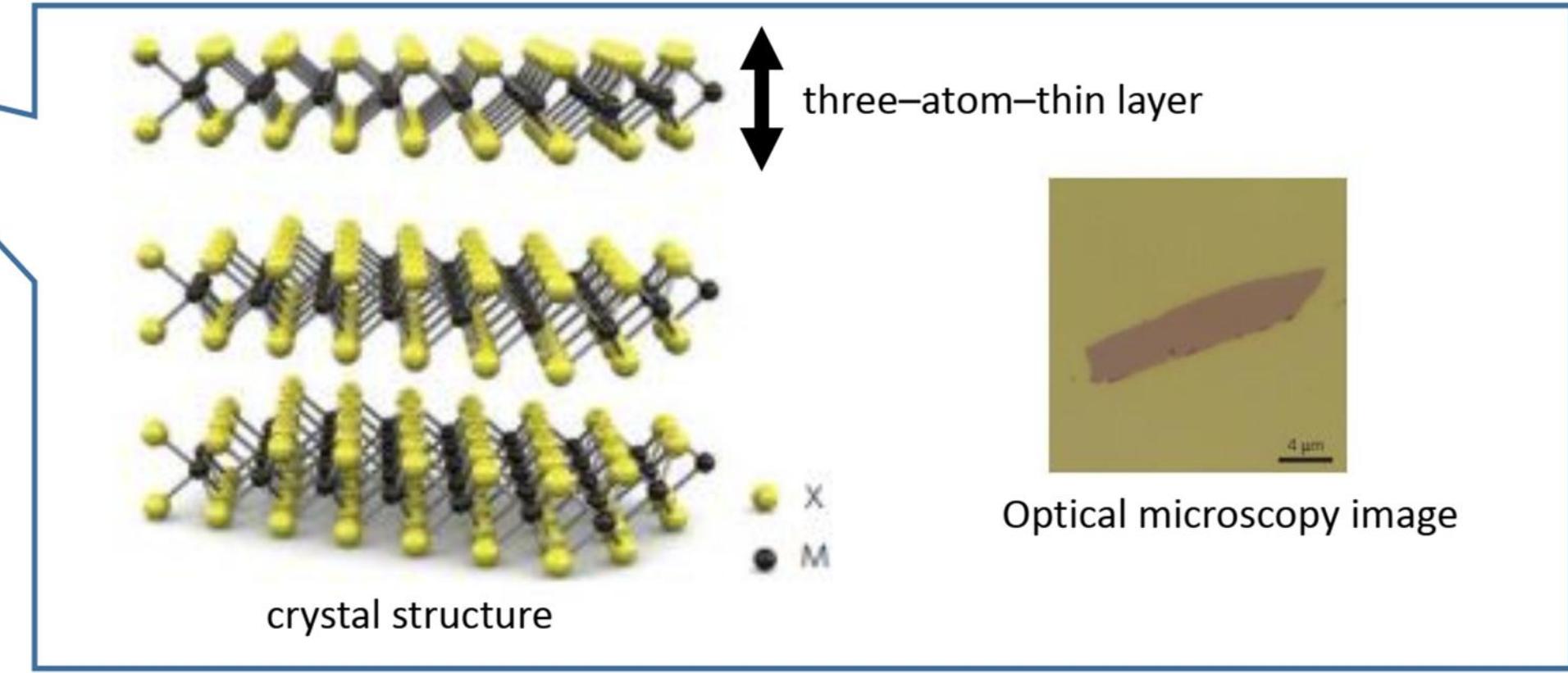


bulk crystal MoS_2



For lubrication

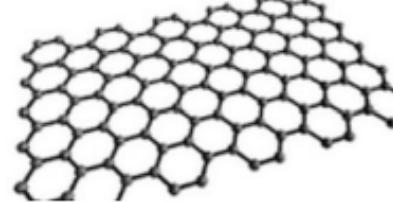
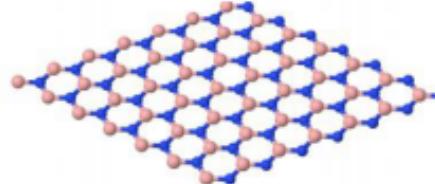
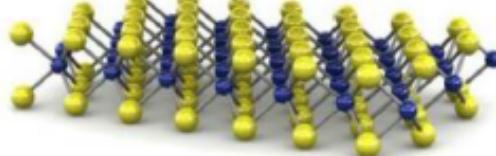
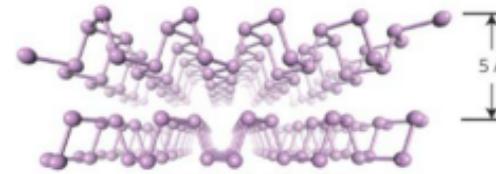
Ampere cop



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

2-D materials

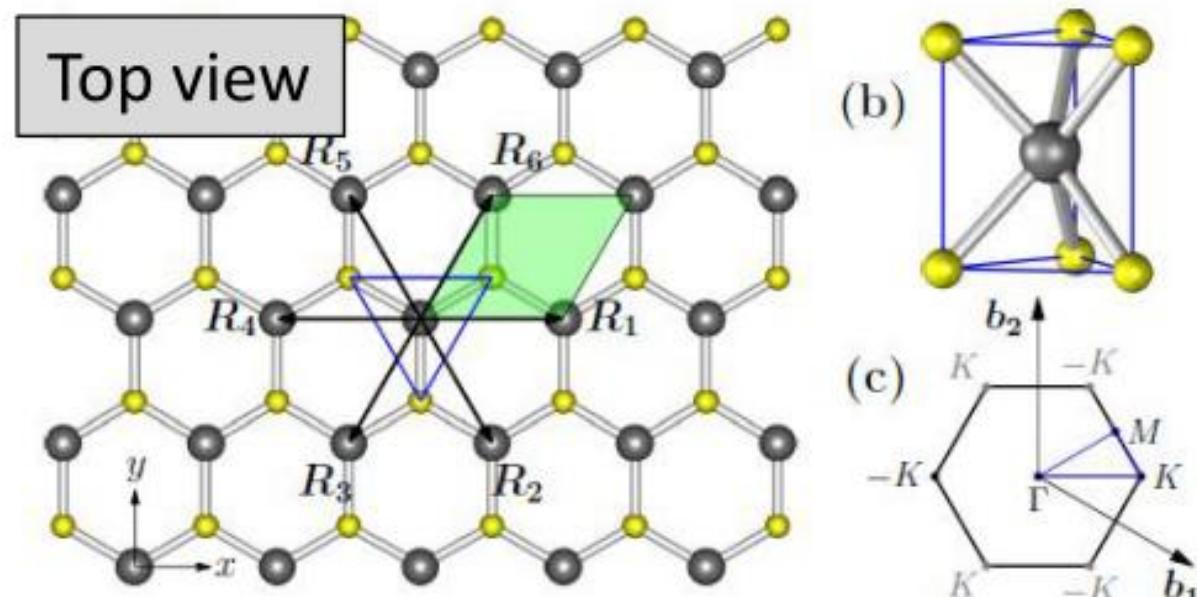
- More than 140 two-dimensional (2-D) materials, and the number is still growing
- Covering insulators, semiconductors, and metals

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)	 5 Å	~2 eV (Monolayer) ~0.3eV (few layer)	100~1000

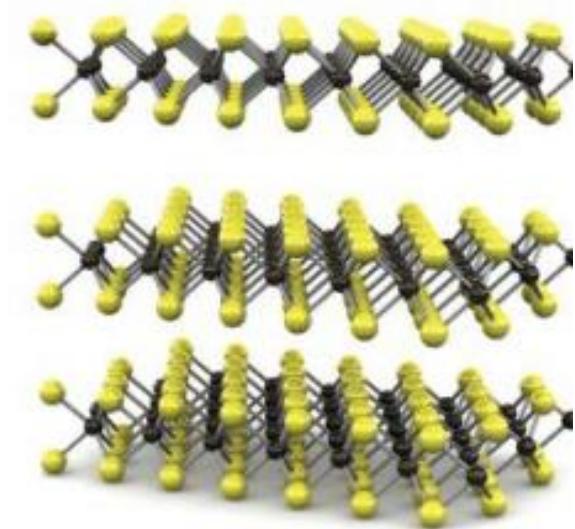
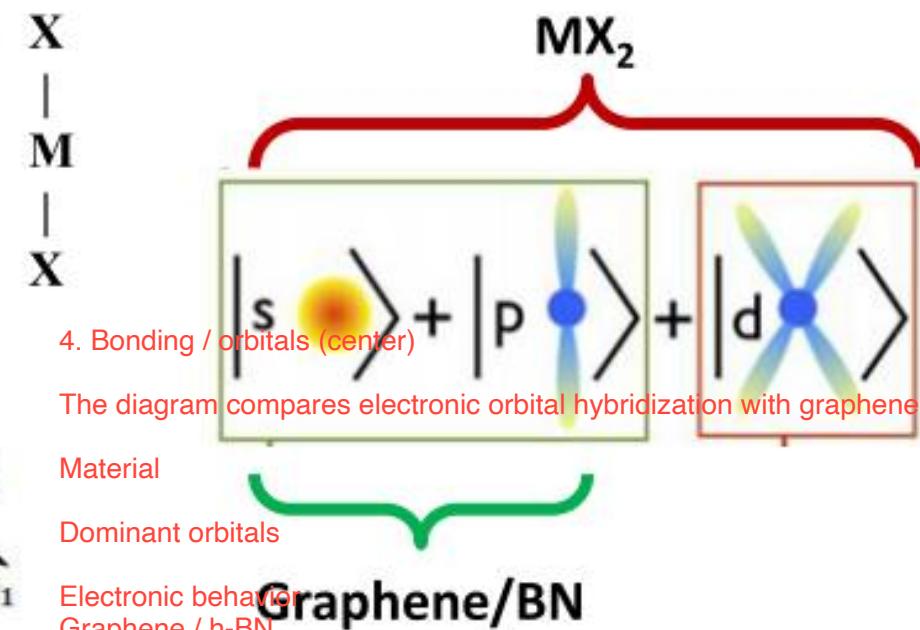
2-D Transition Metal Dichalcogenide

23

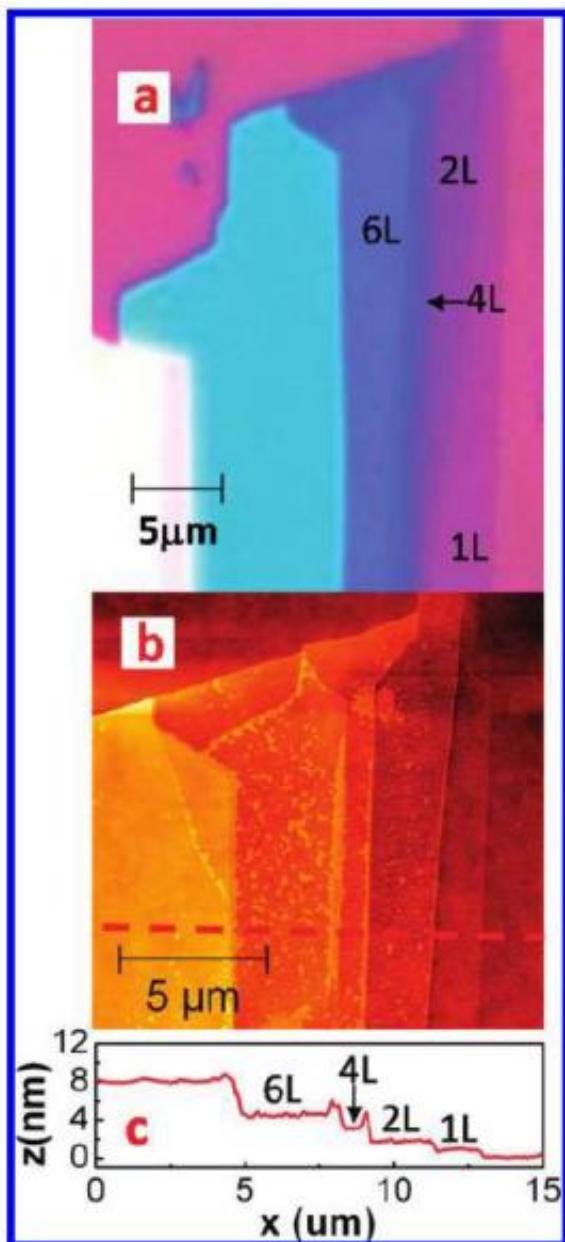
- Lattice structure (1H)



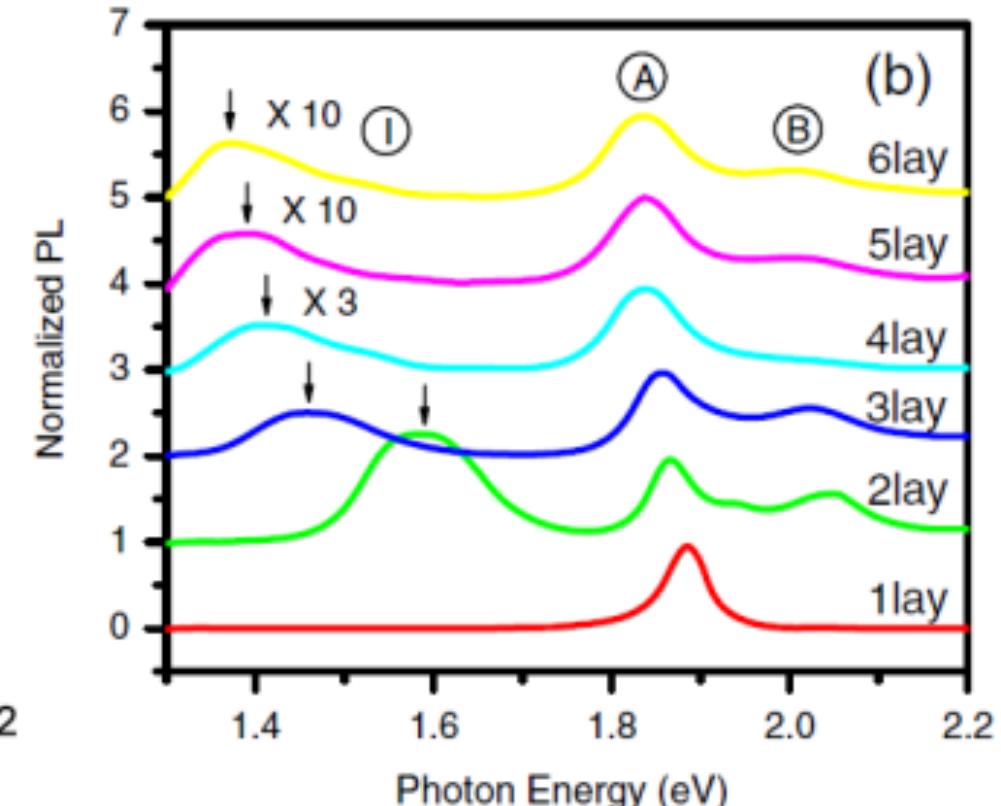
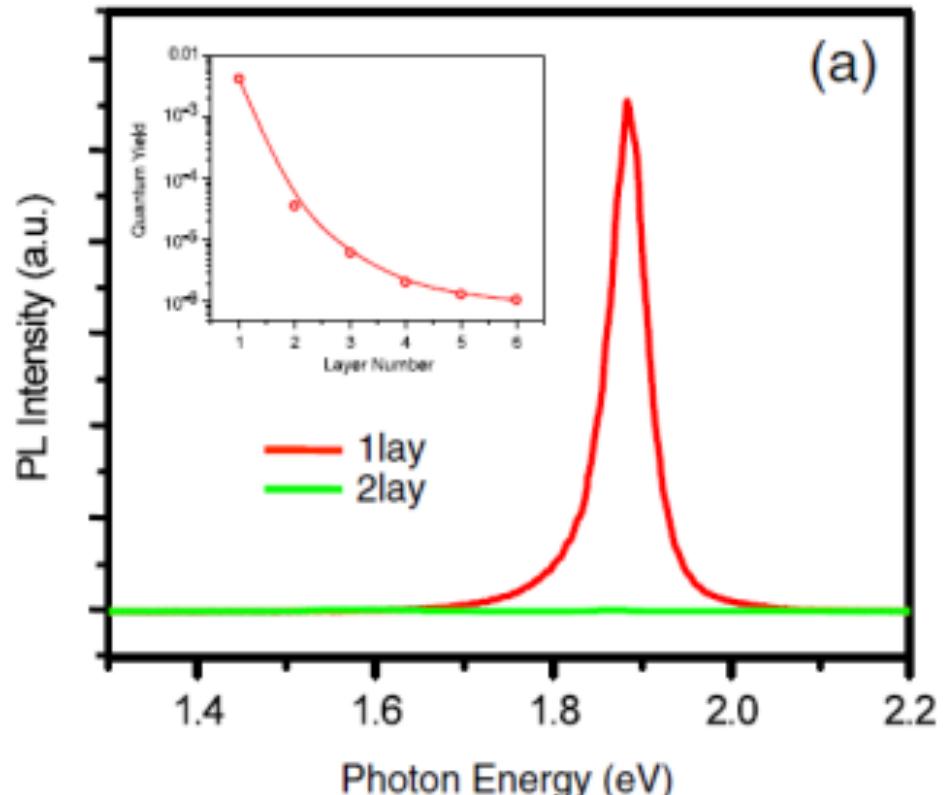
M = Transition metal (Mo, W, etc.)
X = Chalcogen (S, Se, Te)



TMD direct and indirect band gap

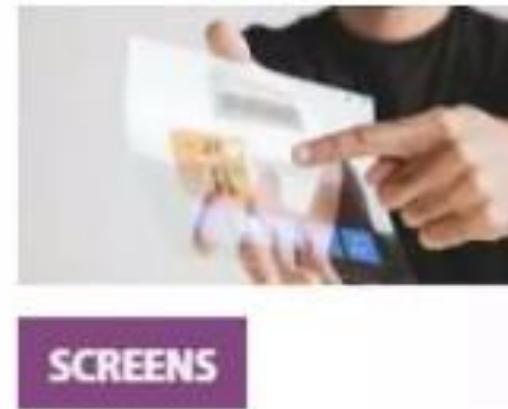


10⁴ times stronger photoluminescence (PL) in 1 layer MoS₂



Applications

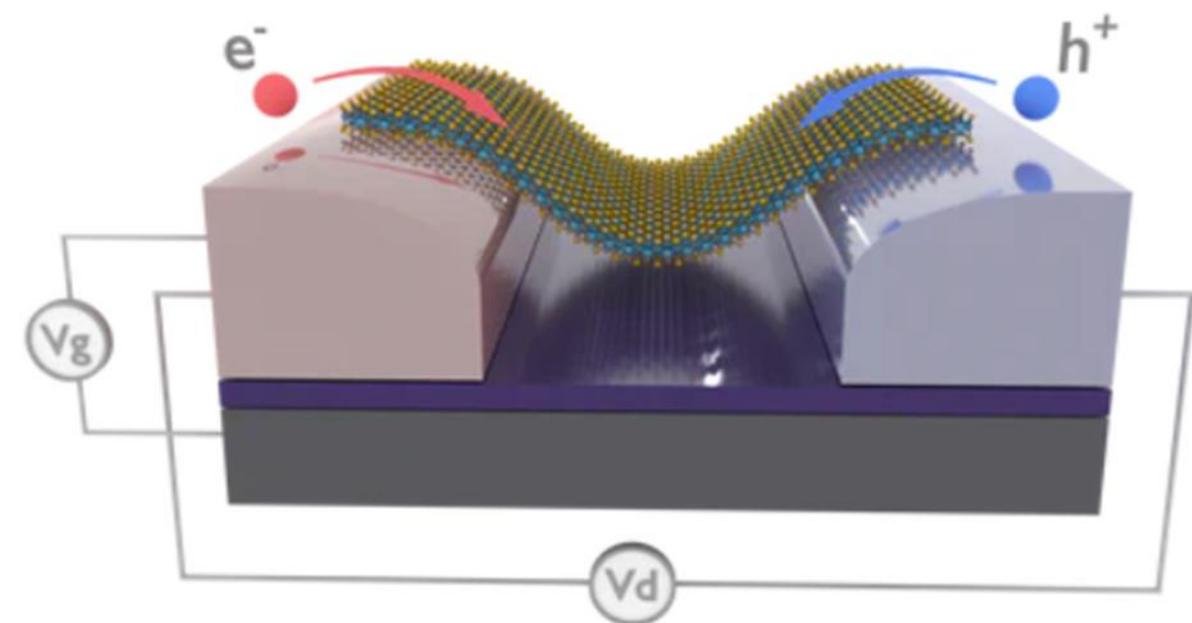
2-D materials have the potential to revolutionize many electronics applications such as solar cells, transistors, camera sensors, digital screens, and semiconductors.



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)

