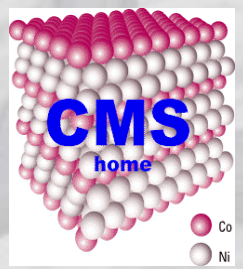
MESA+
INSTITUTE FOR NANOTECHNOLOGY

UNIVERSITY OF TWENTE.

Two-dimensional (2D) materials

Geert Brocks

Computational Materials Science, Fac. Science & Technology,
MESA+ Research Institute for Nanotechnology,
University of Twente, Enschede, Netherlands

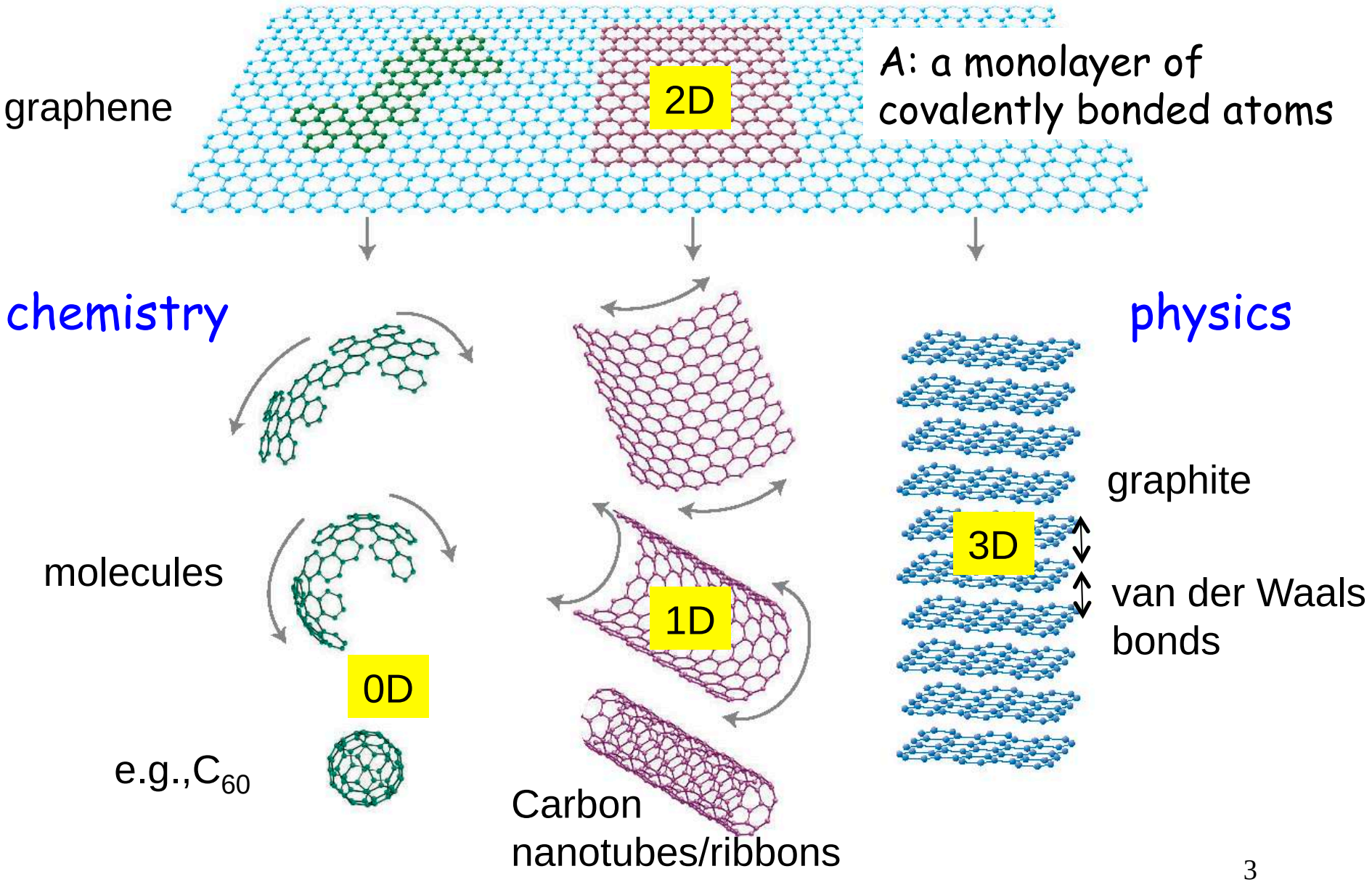


FOM

Introduction

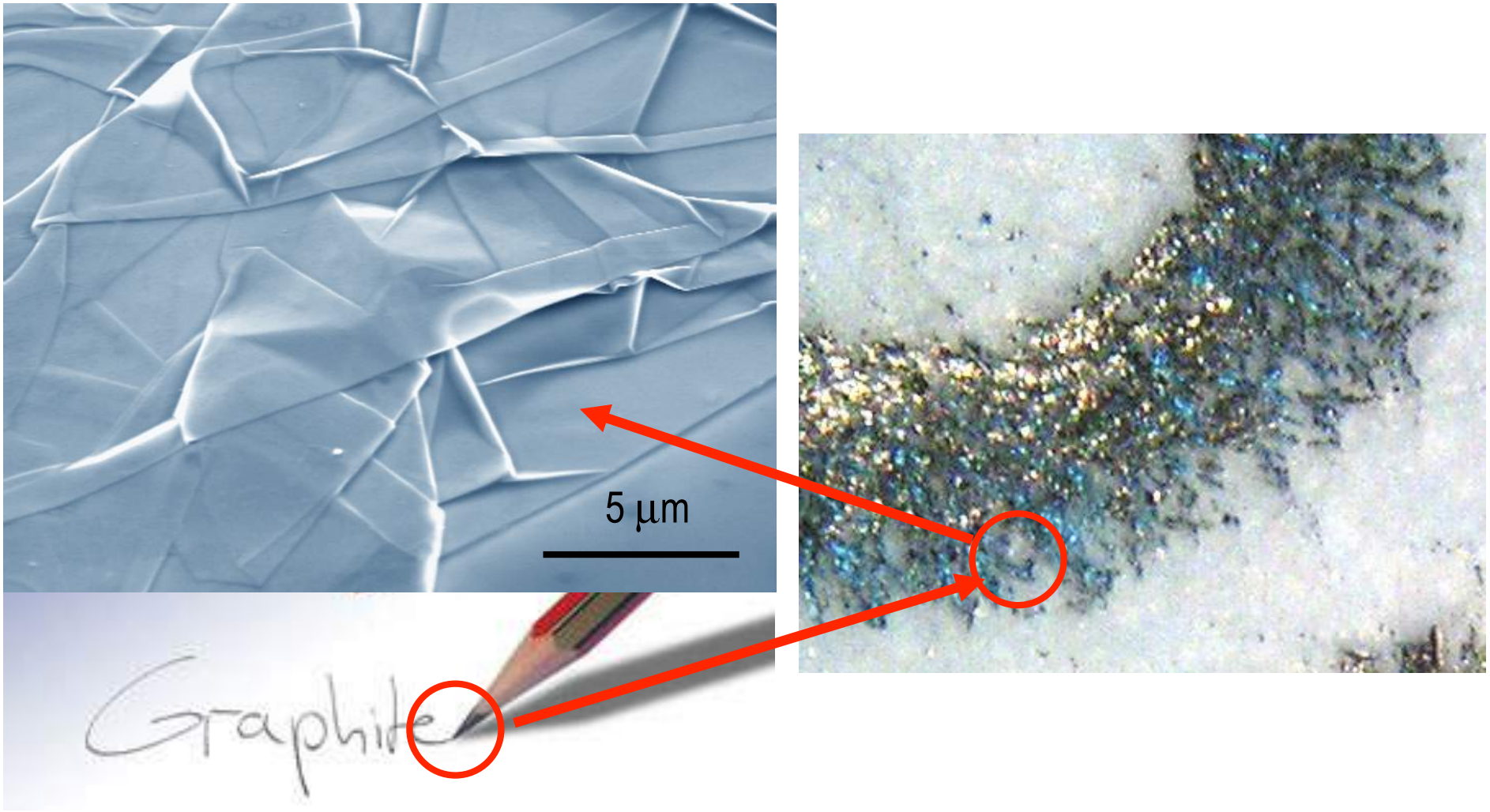
What are two-dimensional (2D) materials ?

Q: what is a 2D material?

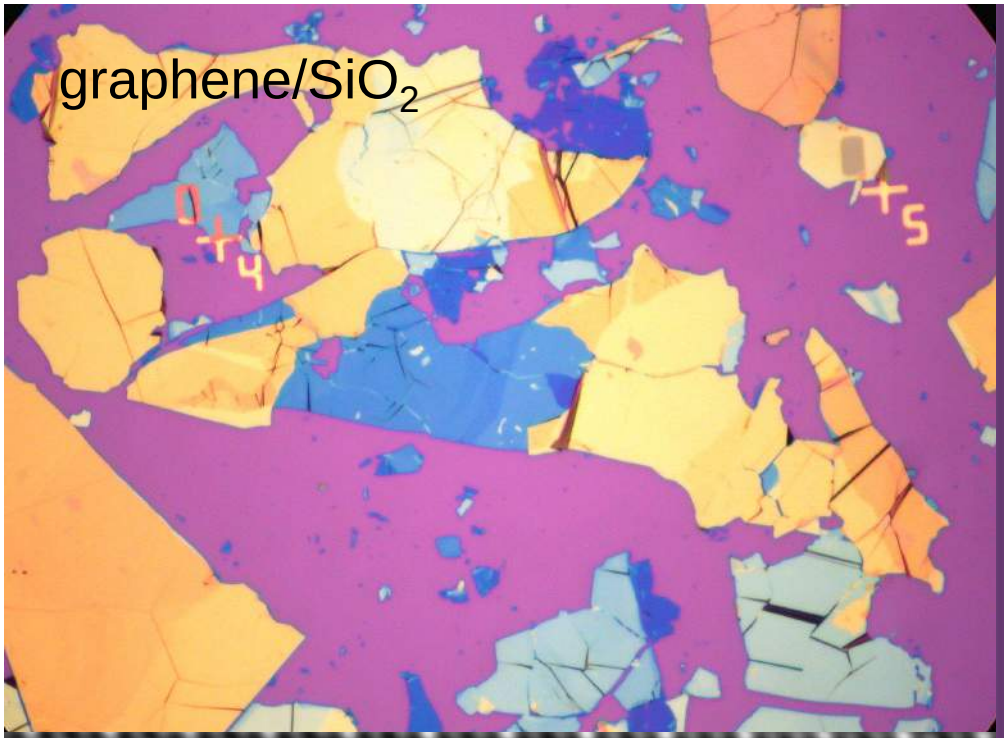


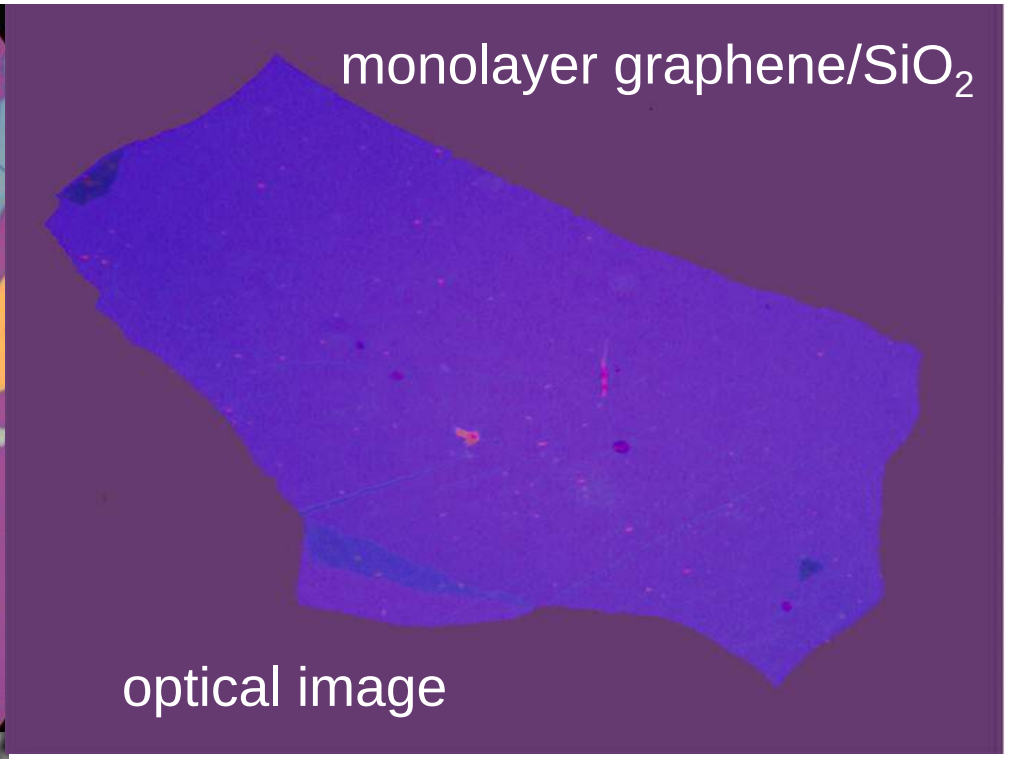
Geim & Novoselov, Nat. Mater. **6**, 183–191 (2007)

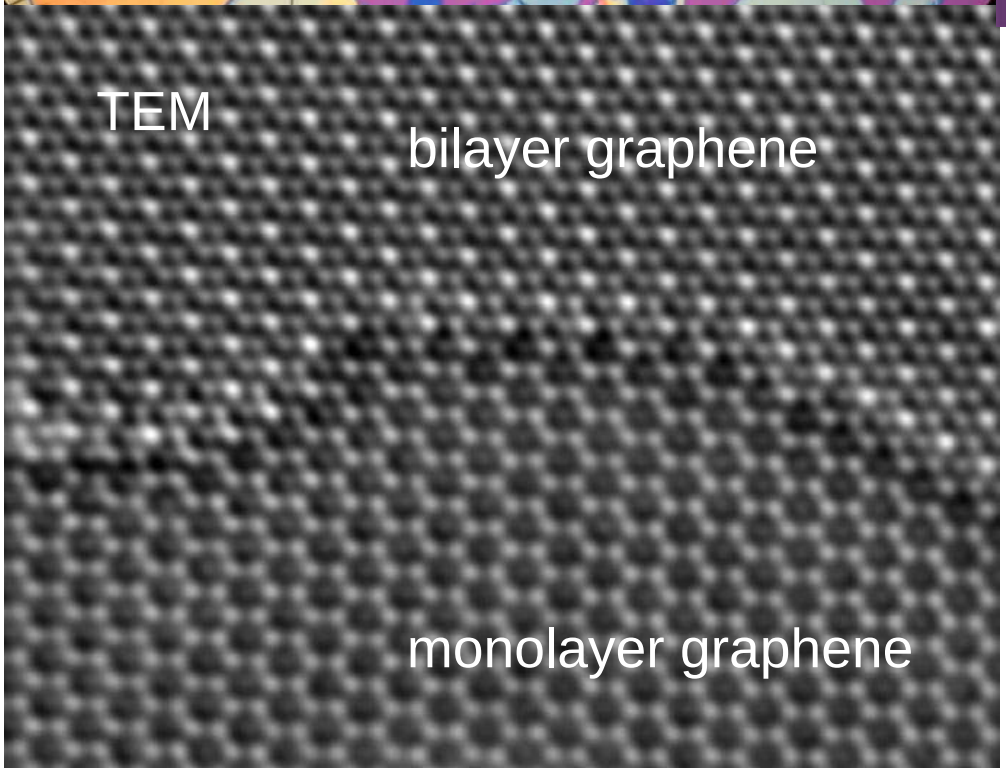
Graphene: a natural material



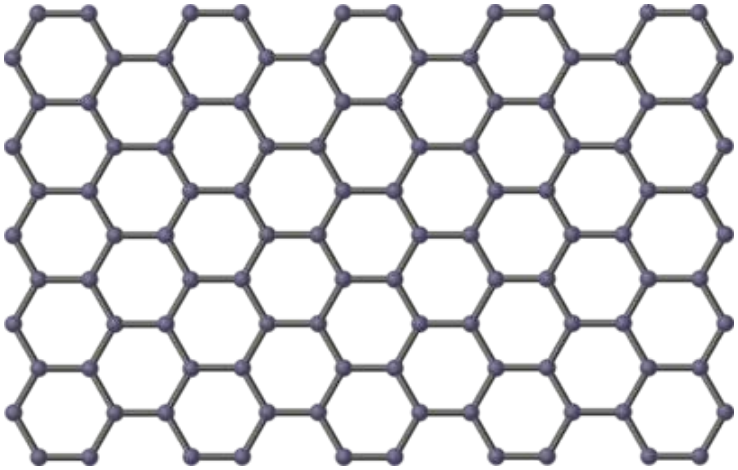
Geim & Novoselov







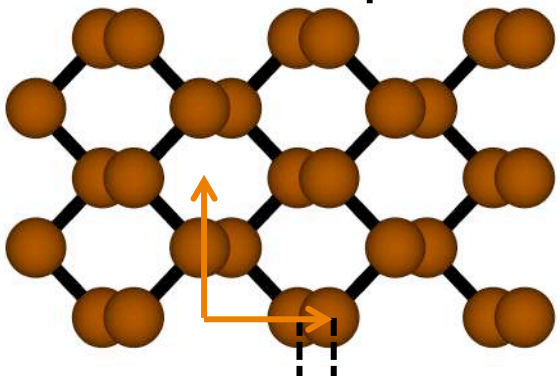
honeycomb lattice C atoms



Jinschek et al., Carbon 49, 556 (2011)

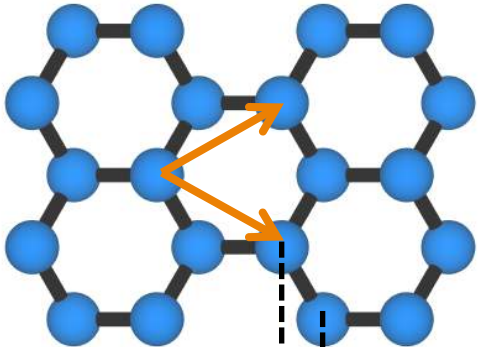
Elemental 2D materials

Black Phosphorus



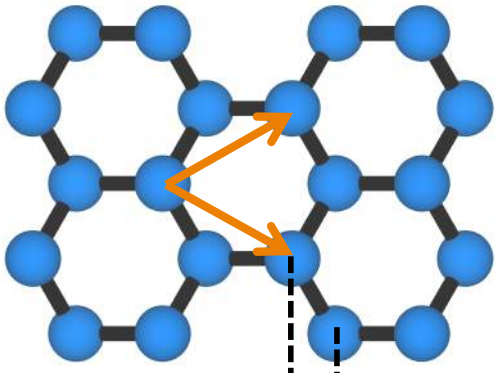
semiconductor

Germanene*

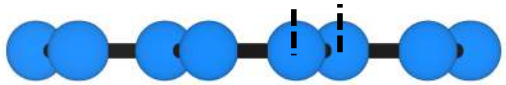


topological insulator?

Graphene



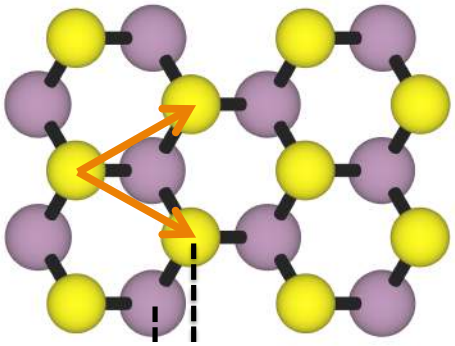
conductor



H 1.0079																	He 4.0026
Li 6.941	Be 9.0122											B 10.811	**C 12.011**	N 14.007	O 15.999	F 18.998	Ne 20.180
Na 22.990	Mg 24.305											Al 26.982	**Si 28.086**	**P 30.974**	S 32.065	Cl 35.453	Ar 39.948
K 39.098	Ca 40.078	Sc 44.956	Ti 47.867	V 50.942	Cr 51.996	Mn 54.938	Fe 55.845	Co 58.933	Ni 58.693	Cu 63.546	Zn 65.38	Ga 69.723	**Ge 72.64**	As 74.922	Se 78.96	Br 79.904	Kr 83.798
Rb 85.468	Sr 87.62	Y 88.906	Zr 91.224	Nb 92.906	Mo 95.96	Tc [98]	Ru 101.07	Rh 102.91	Pd 106.42	Ag 107.87	Cd 112.41	In 114.82	Sn 118.71	Sb 121.76	Te 127.60	I 126.90	Xe 131.29
Cs 132.91	Ba 137.33		Hf 178.49	Ta 180.95	W 183.84	Re 186.21	Os 190.23	Ir 192.22	Pt 195.08	Au 196.97	Hg 200.59	Tl 204.38	Pb 207.2	Bi 208.98	Po [209]	At [210]	^{6}Rn [222]

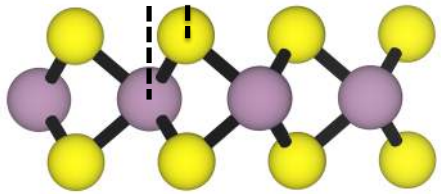
* A. Acun, et al., J. Phys.: CM 27, 443002 (2015)

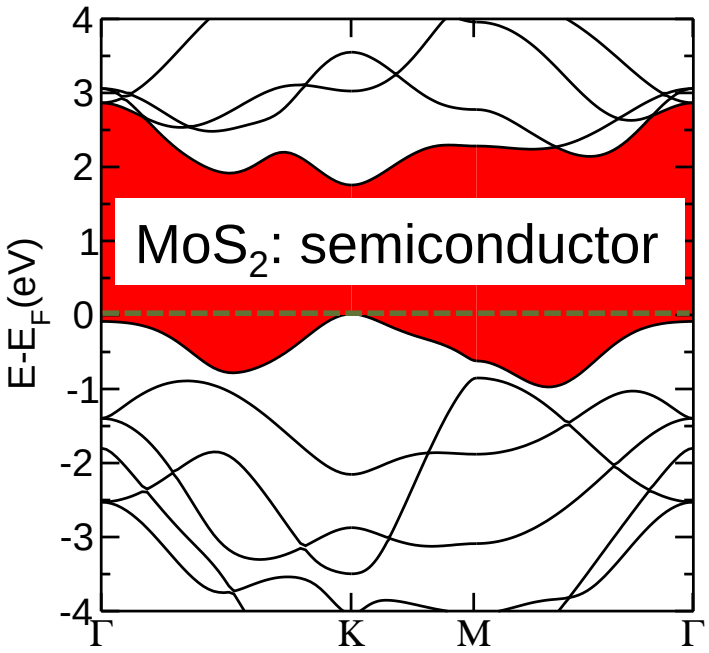
Compound 2D materials: MX_2

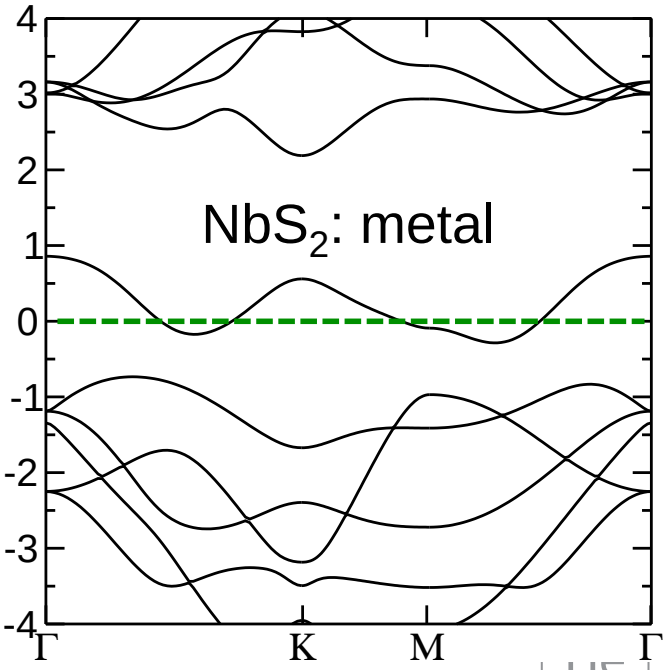


trilayer

X
M
X



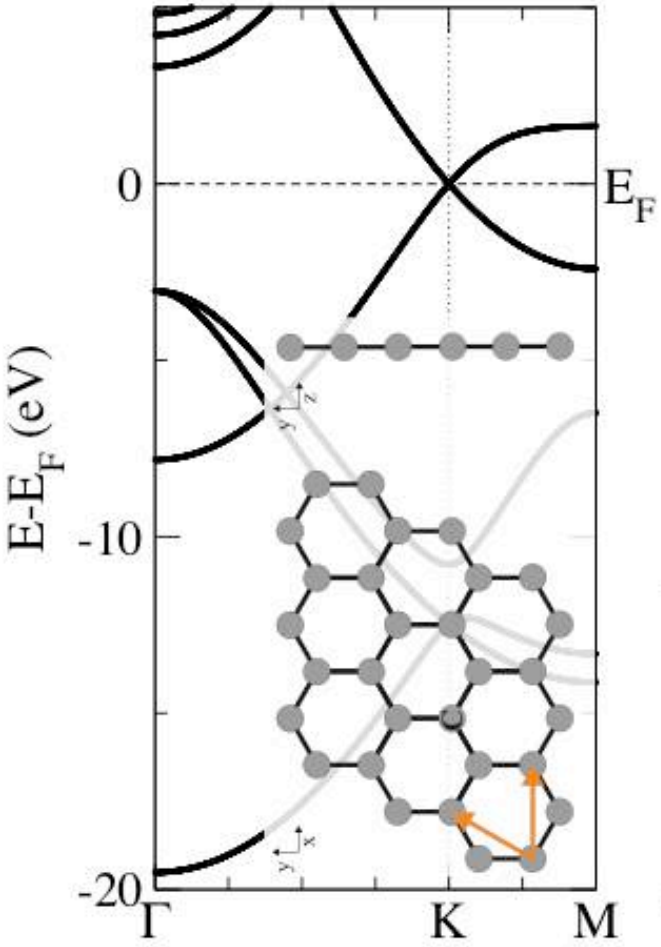




H 1.0079																	He 4.0026
lithium 3 Li 6.941	beryllium 4 Be 9.0122											boron 5 B 10.811	carbon 6 C 12.011	nitrogen 7 N 14.007	oxygen 8 O 15.999	fluorine 9 F 18.998	neon 10 Ne 20.180
sodium 11 Na 22.990	magnesium 12 Mg 24.305											aluminium 13 Al 26.982	silicon 14 Si 28.086	phosphorus 15 P 30.974	**sulfur 16 S 32.065**	chlorine 17 Cl 35.453	argon 18 Ar 39.948
potassium 19 K 39.098	calcium 20 Ca 40.078	scandium 21 Sc 44.956	titanium 22 Ti 47.867	**vanadium 23 V 50.942**	chromium 24 Cr 51.996	manganese 25 Mn 54.938	iron 26 Fe 55.845	cobalt 27 Co 58.933	nickel 28 Ni 58.693	copper 29 Cu 63.546	zinc 30 Zn 65.38	gallium 31 Ga 69.723	germanium 32 Ge 72.64	arsenic 33 As 74.922	**selenium 34 Se 78.96**	bromine 35 Br 79.904	krypton 36 Kr 83.798
rubidium 37 Rb 85.468	strontium 38 Sr 87.62	yttrium 39 Y 88.906	zirconium 40 Zr 91.224	**niobium 41 Nb 92.906**	**molybdenum 42 Mo 95.96**	technetium 43 Tc [98]	ruthenium 44 Ru 101.07	rhodium 45 Rh 102.91	palladium 46 Pd 106.42	silver 47 Ag 107.87	cadmium 48 Cd 112.41	indium 49 In 114.82	tin 50 Sn 118.71	antimony 51 Sb 121.76	**tellurium 52 Te 127.60**	iodine 53 I 126.90	xenon 54 Xe 131.29
caesium 55 Cs 132.91	barium 56 Ba 137.33		hafnium 72 Hf 178.49	**tantalum 73 Ta 180.95**	**tungsten 74 W 183.84**	rhenium 75 Re 186.21	osmium 76 Os 190.23	iridium 77 Ir 192.22	platinum 78 Pt 195.08	gold 79 Au 196.97	mercury 80 Hg 200.59	thallium 81 Tl 204.38	lead 82 Pb 207.2	bismuth 83 Bi 208.98	polonium 84 Po [209]	astatine 85 At [210]	radon 86 Rn [222]

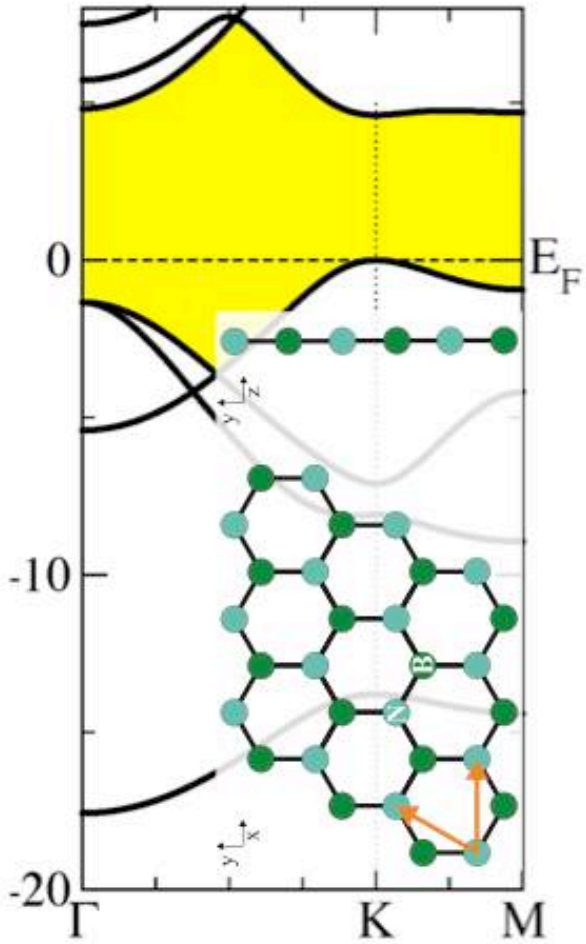
Honeycomb lattices

graphene



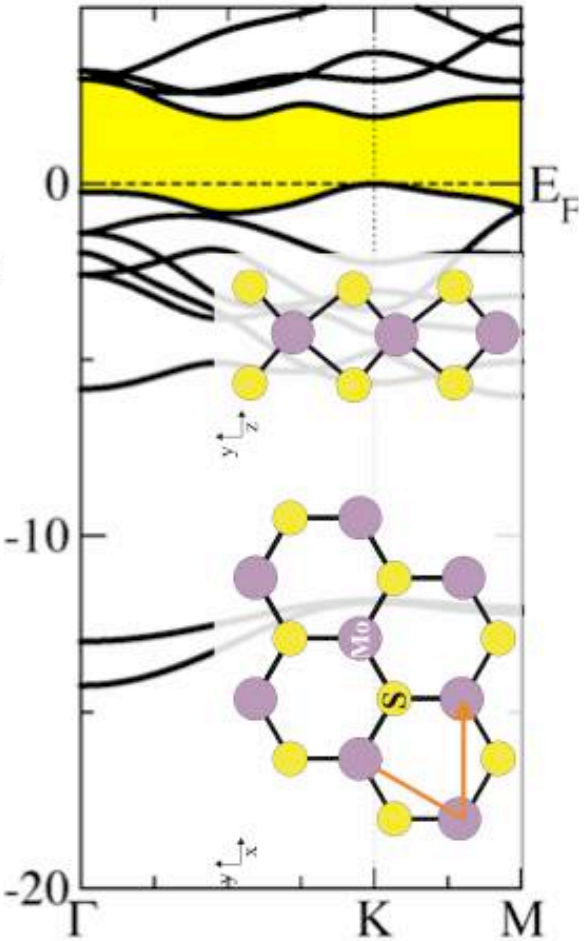
(semi)metal

boron nitride



insulator

MoS_2

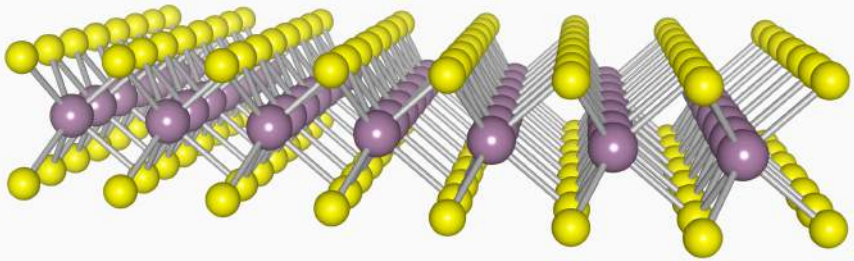


semiconductor

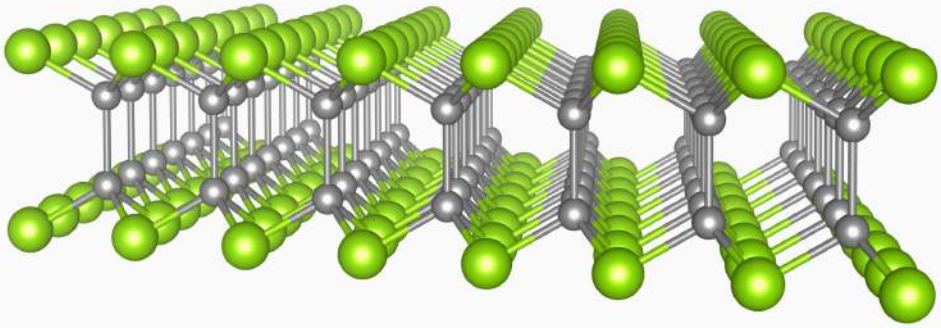
M. Bokdam, thesis, U Twente (2013); M. Bokdam, GB, NTvN, 282 (2014)

2D lattices

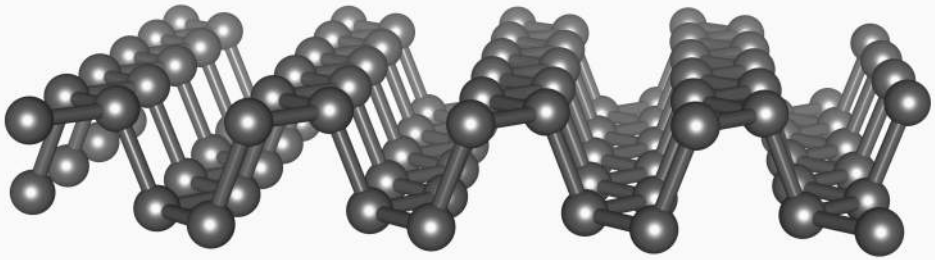
MoS_2



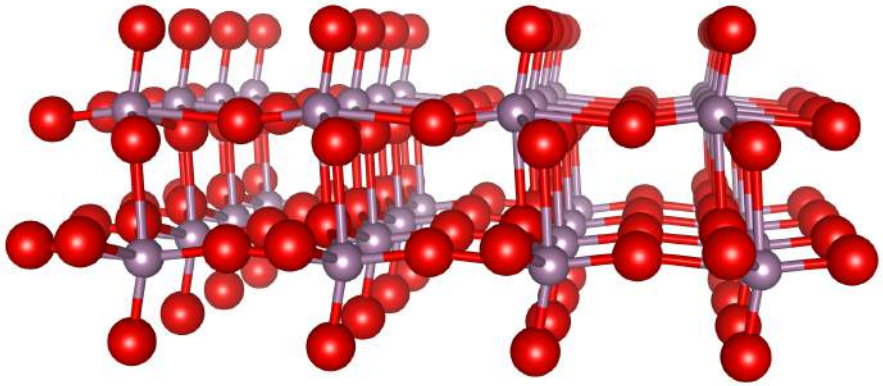
GaSe



black P



MoO_3



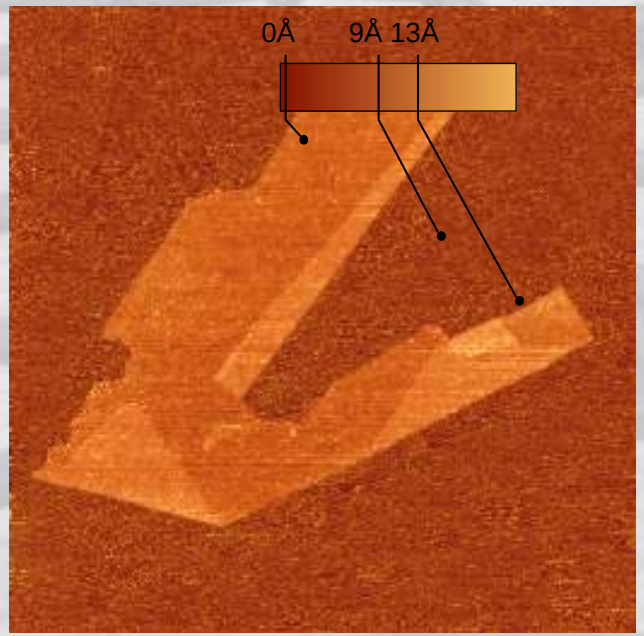
all are neutral, closed shell 2D layers

Introduction

What can we do with two-dimensional (2D) materials?

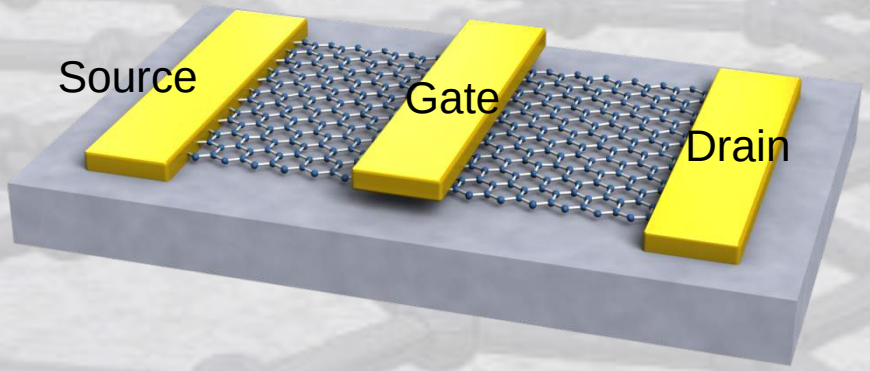
The rise of 2D materials

graphene



Novoselov, Geim, et al.,
Science **306**, 666 (2004)

Field Effect Transistor (FET)



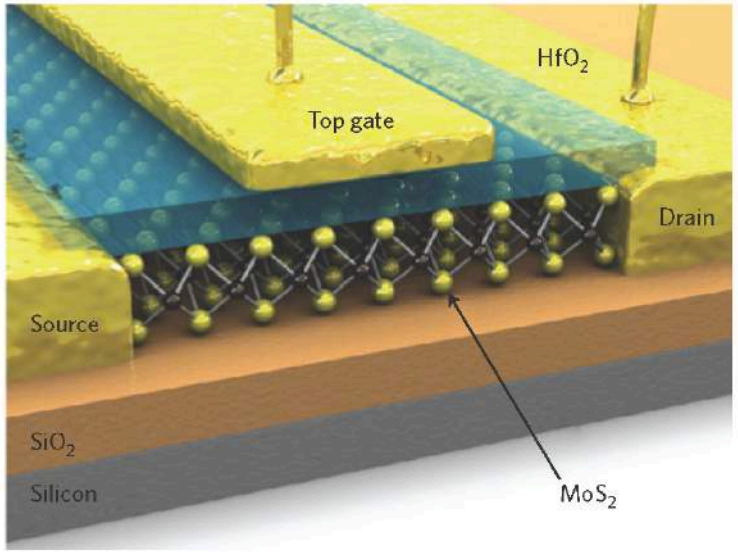
- very high carrier mobility $\mu \approx 10^5\ \mathrm{cm}^2/(\mathrm{Vs})$
- quantum Hall effect at room temperature
- "relativistic" effects (Klein tunneling)
- ... more and more ...

physics Nobel prize 2010: Andre Geim & Konstantin Novoselov

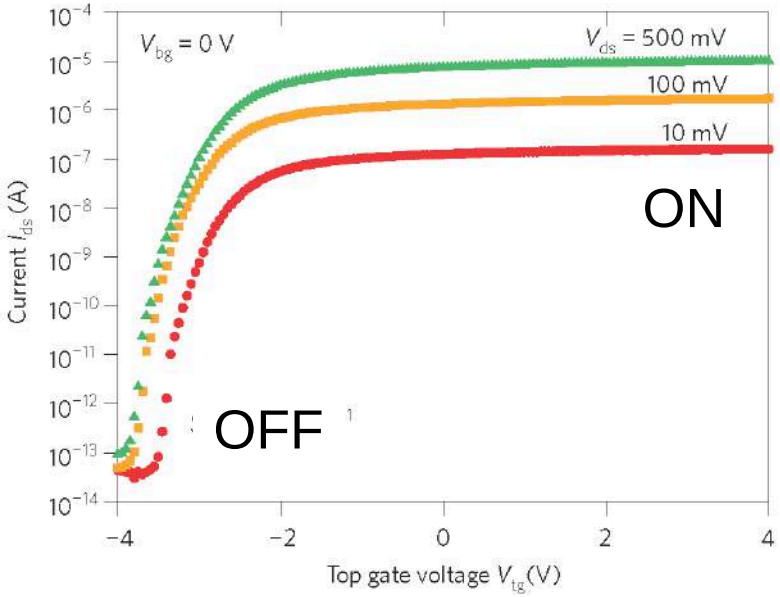
"for groundbreaking experiments regarding the two-dimensional material graphene"

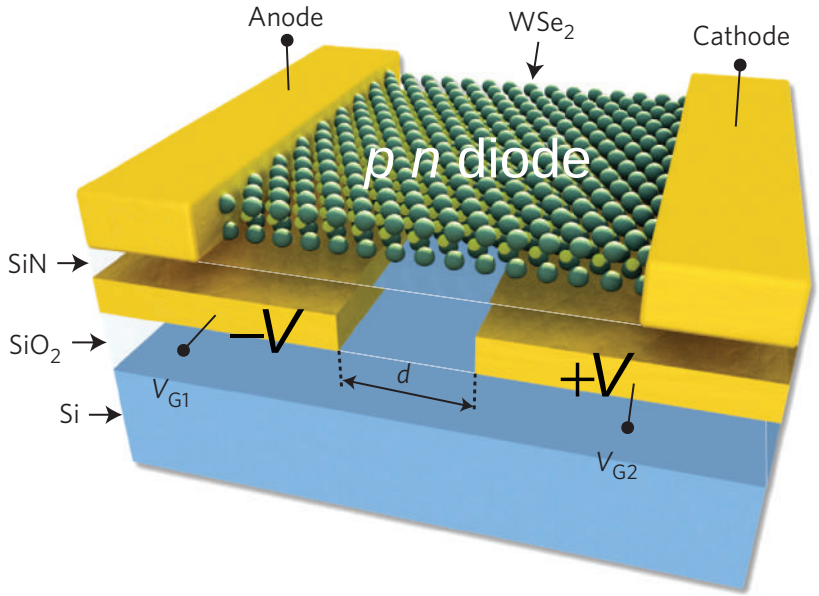
Application: (opto)electronics

Wang et al., Nat. Nanotech. 7, 699 (2012)

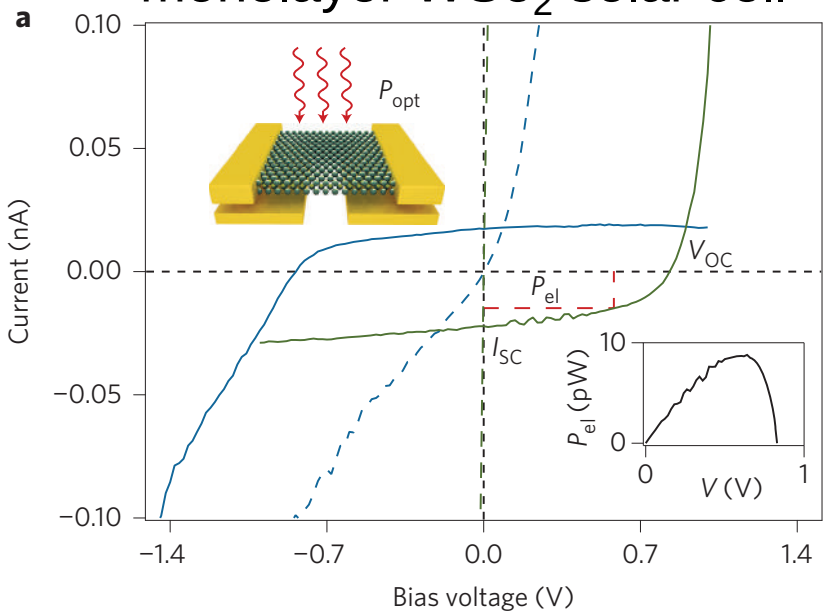


monolayer MoS_2 FETransistor





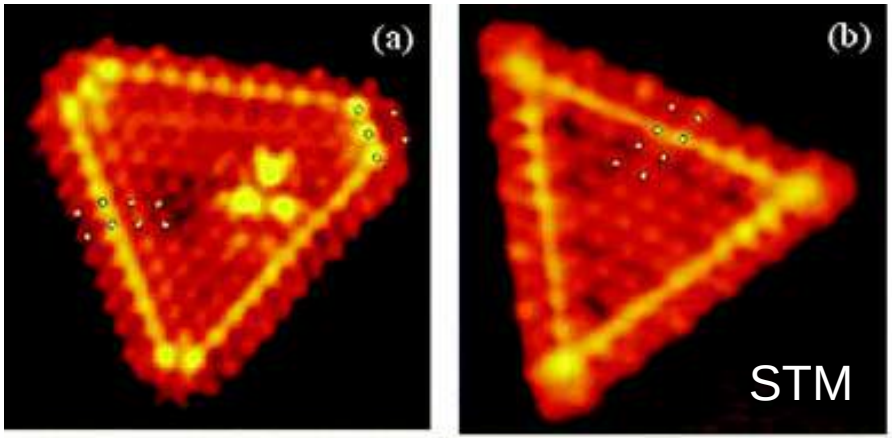
monolayer WSe_2 solar cell



Pospischil et al., Nat. Nanotech. 9, 257 (2014)

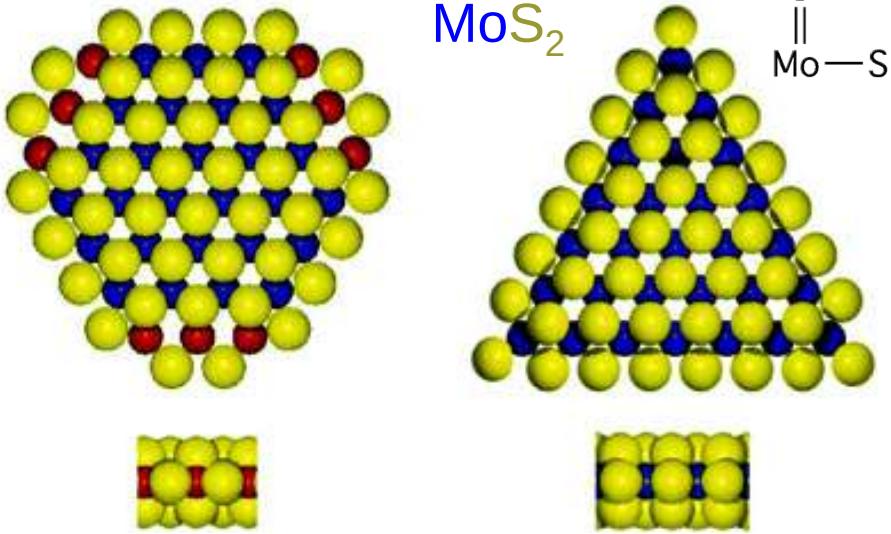
Application: catalysis

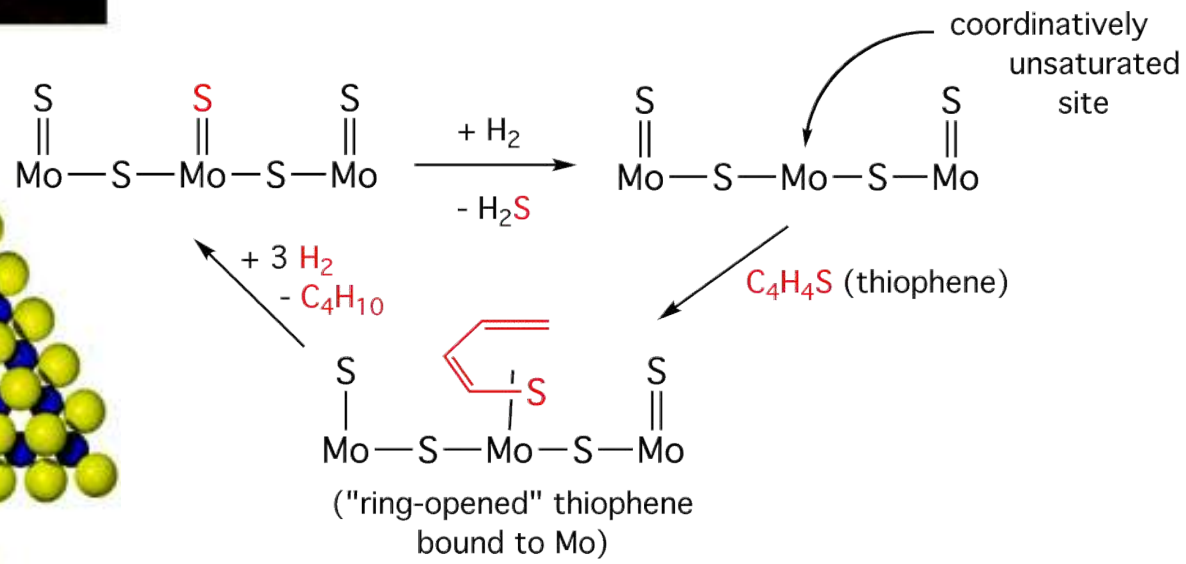
Lauritsen et al., J. Catal. 197, 1 (2001)



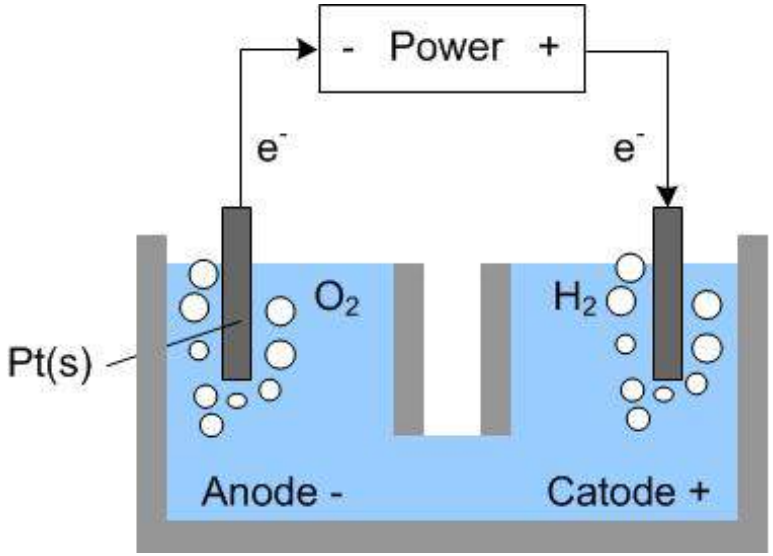
edges of MoS_2 layers are catalytically active

de-sulfurezation

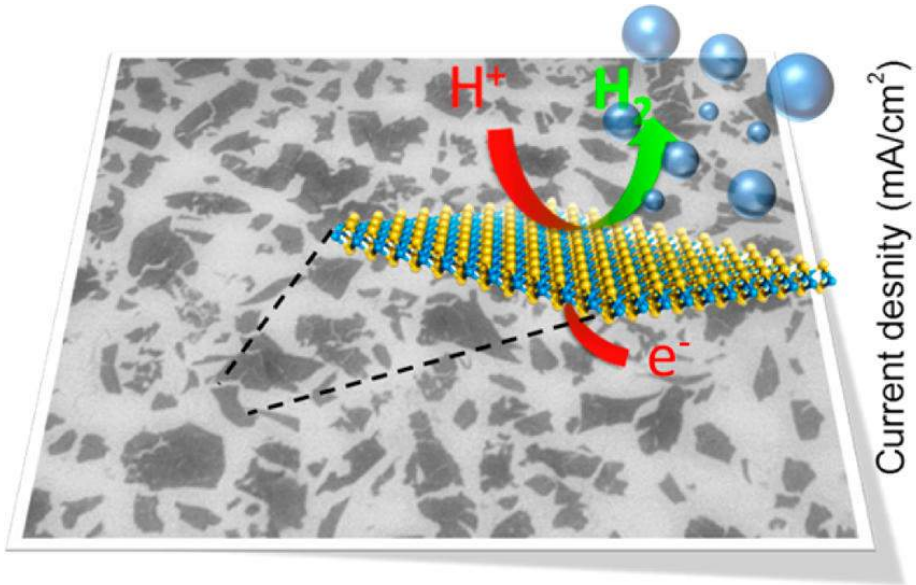


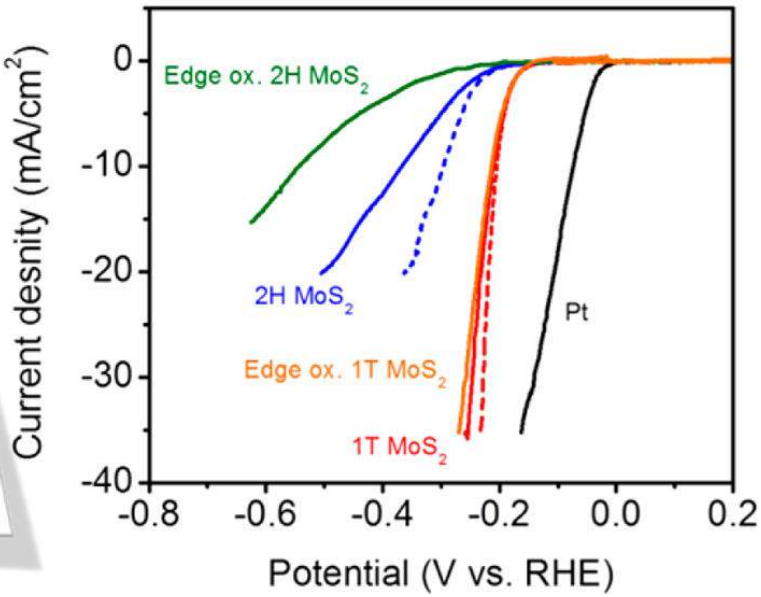


Application: electrolysis



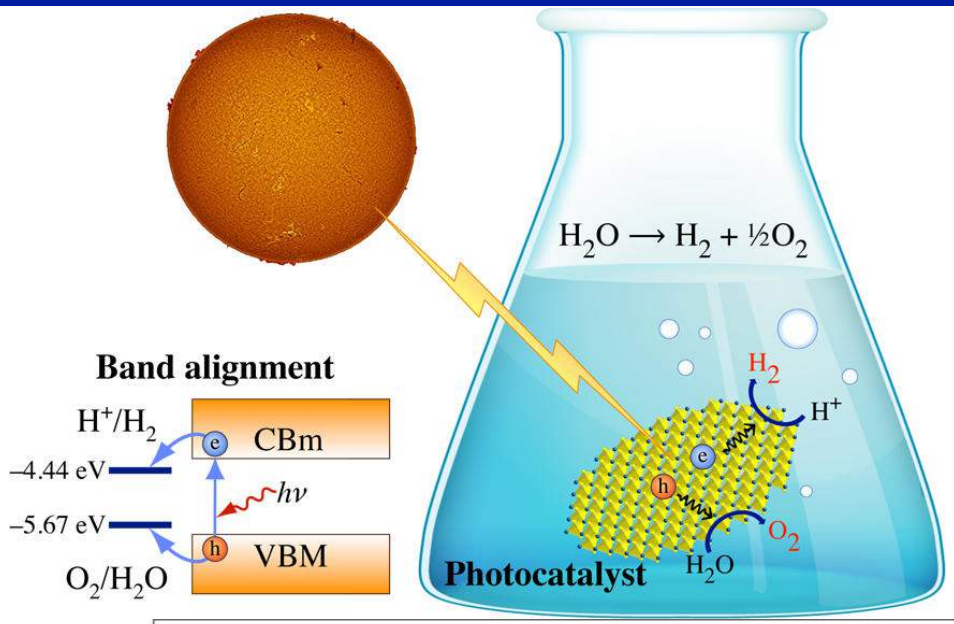
MoS_2 layers good cathode material for hydrogen evolution reaction





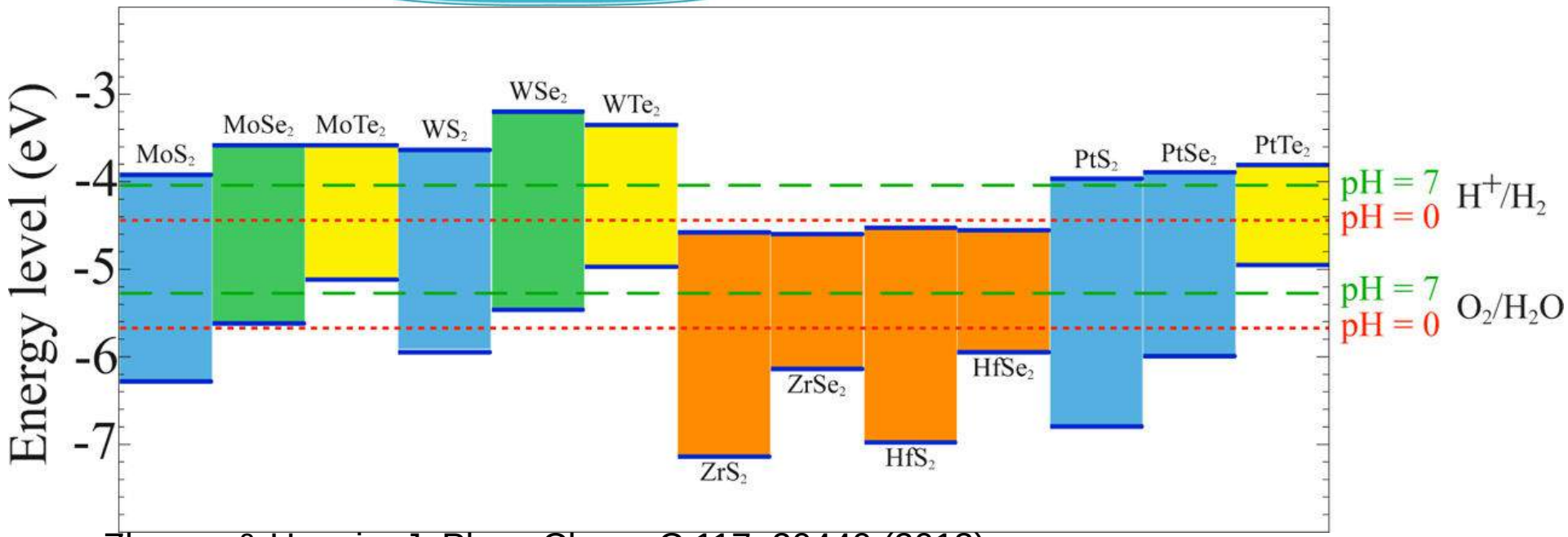
Voiry et al., Nano Lett. 13, 6222 (2013)

Application: solar fuels



MX_2 layers can be good photocatalysts

for making solar fuels: convert photons directly into chemicals



Zhuang & Hennig, J. Phys. Chem. C 117, 20440 (2013)

Summary applications

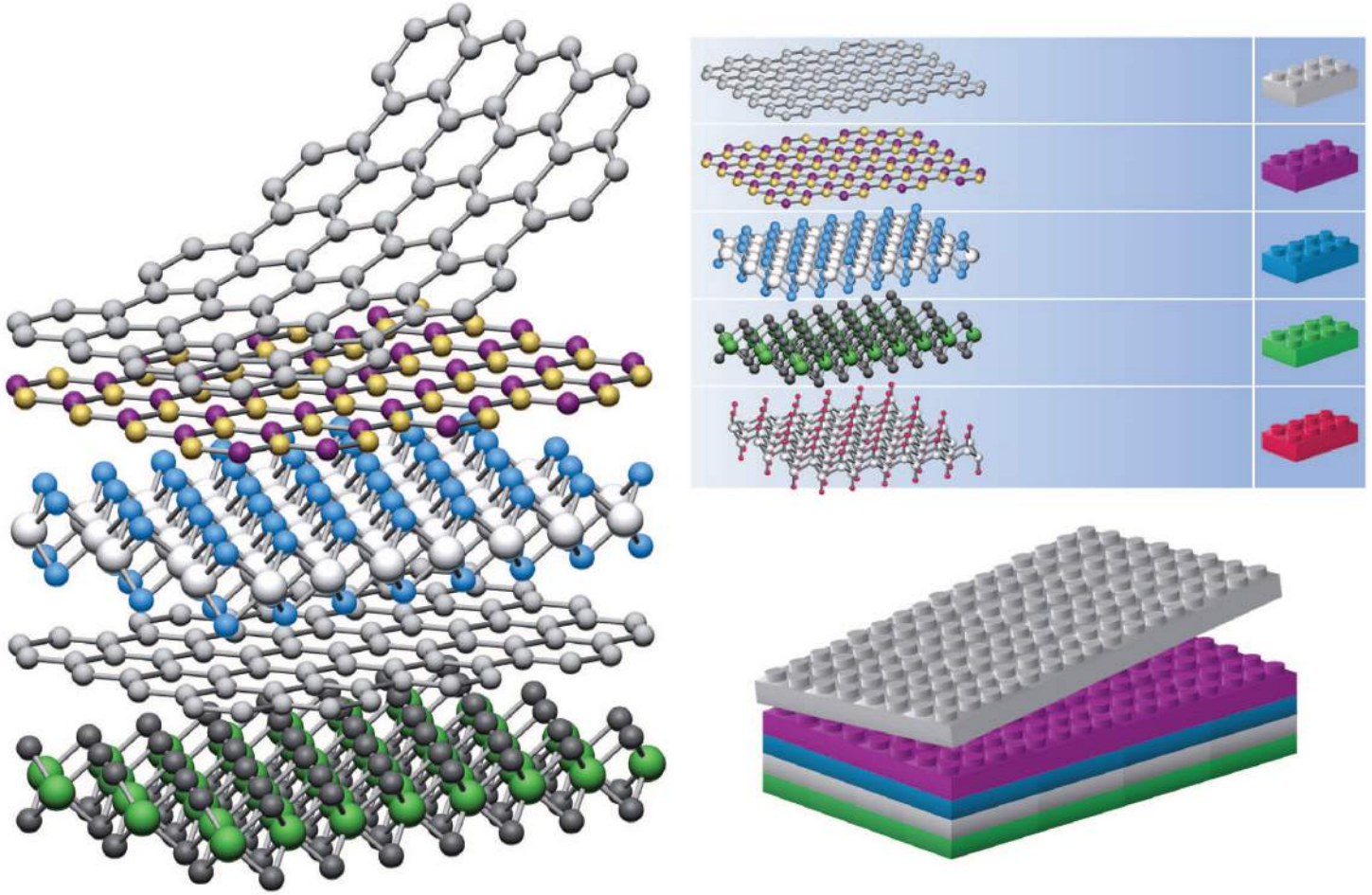
What can we do with
two-dimensional (2D) materials?

- electronic devices
- solar cells (convert photons to electricity)
- catalysis
- electrolysis (convert electricity to fuels)
- solar fuels (convert photons to fuels)

van der Waals heterostructures of 2D materials

combine functionalities of different 2D materials

Geim & Grigorieva, Nature **499,** 419 (2013)



van der Waals heterostructures of 2D materials

combine functionalities of different 2D materials

Novoselov et al., Nature **490,** 192 (2012)