Minicurso 3:

Materiais Bidimensionais

Prof. Lídia C. Gomes

Dia 1 (29/01)

General introduction.

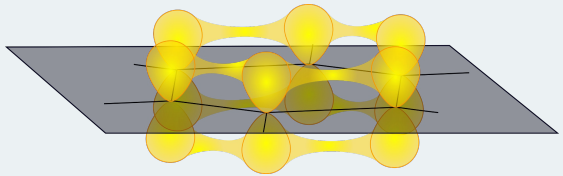
What are 2D materials?

A tiny bit of history.

Some interesting properties.

Dia 2 (30/01)

The origin of dimensionality: an analysis of orbital hybridization in graphene.



Dia 3 (31/01)

Synthesis methods.

Some experimental achievements.

Some help from computers: ML discovery and development of new 2D materials.

2004-2007 Licenciatura em Física - PUC MG

2008-2010 Mestrado em Física - UFMG

2010-2014 Doutorado em Física - UFMG

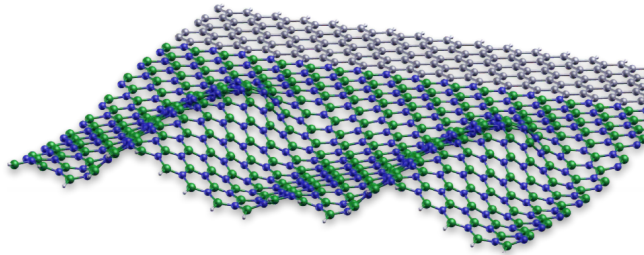
2014-2017 Pós-Doutorado - CA2DM, NUS

NUS National University of Singapore | Centre for Advanced 2D Materials

2017-2019 Pós-Doutorado - NCSA, UIUC

2020-2021 Pós-Doutorado - UIUC + IFT, UNESP

2022 Profa Adjunta - UFPE

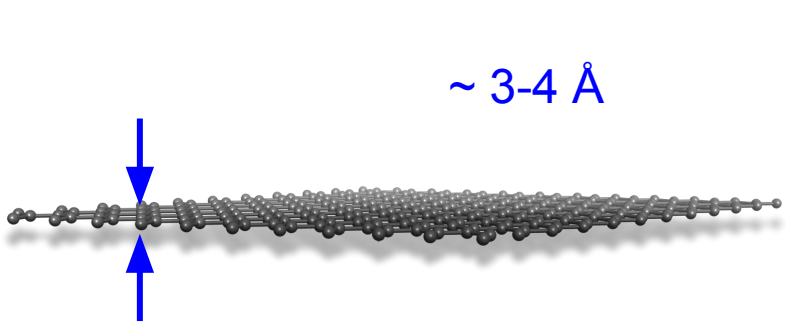


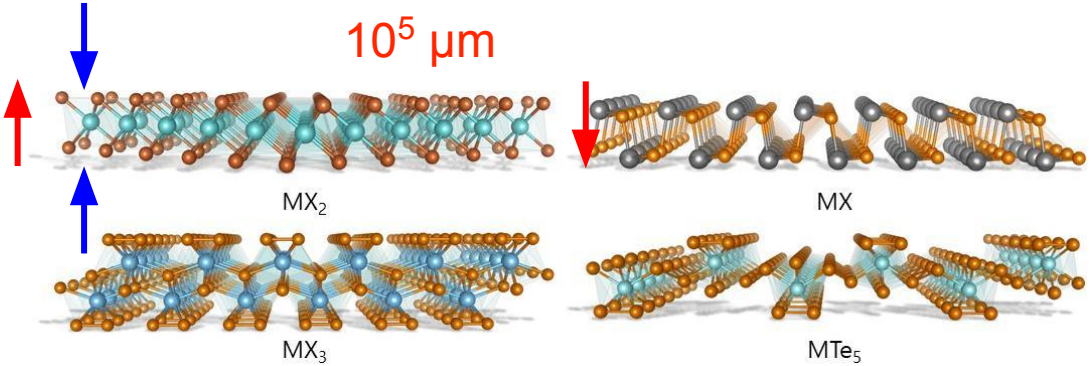
Materiais ~~bidimensionais~~ atomicamente finos

O que são?

Cristais com um ou poucos átomos de espessura

Interações eletrônicas no plano são muito mais fortes do que aquelas na direção perpendicular ao plano.





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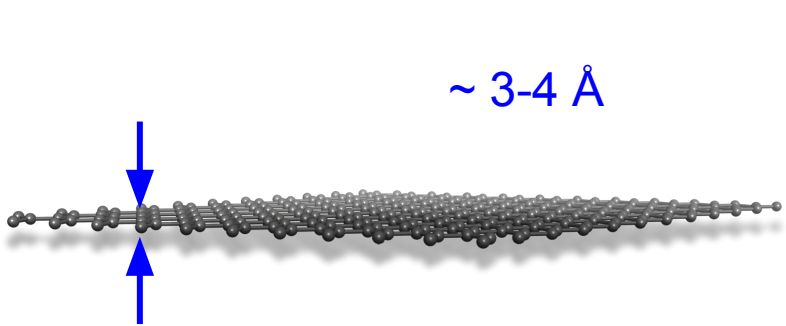
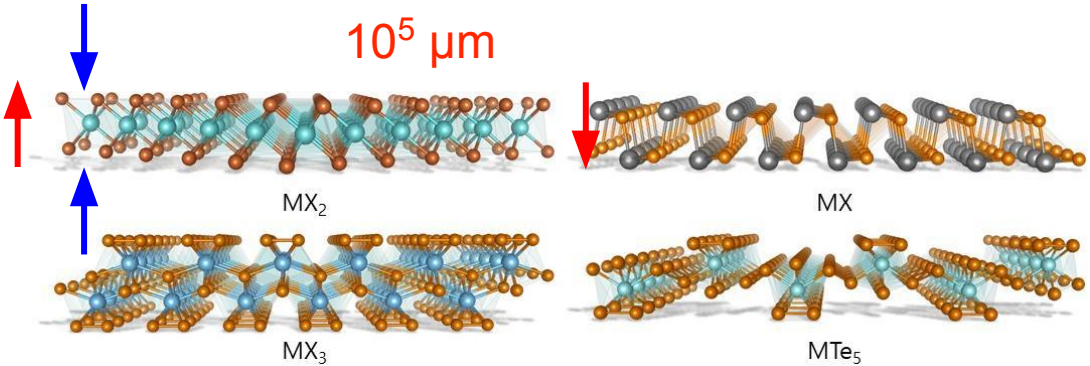
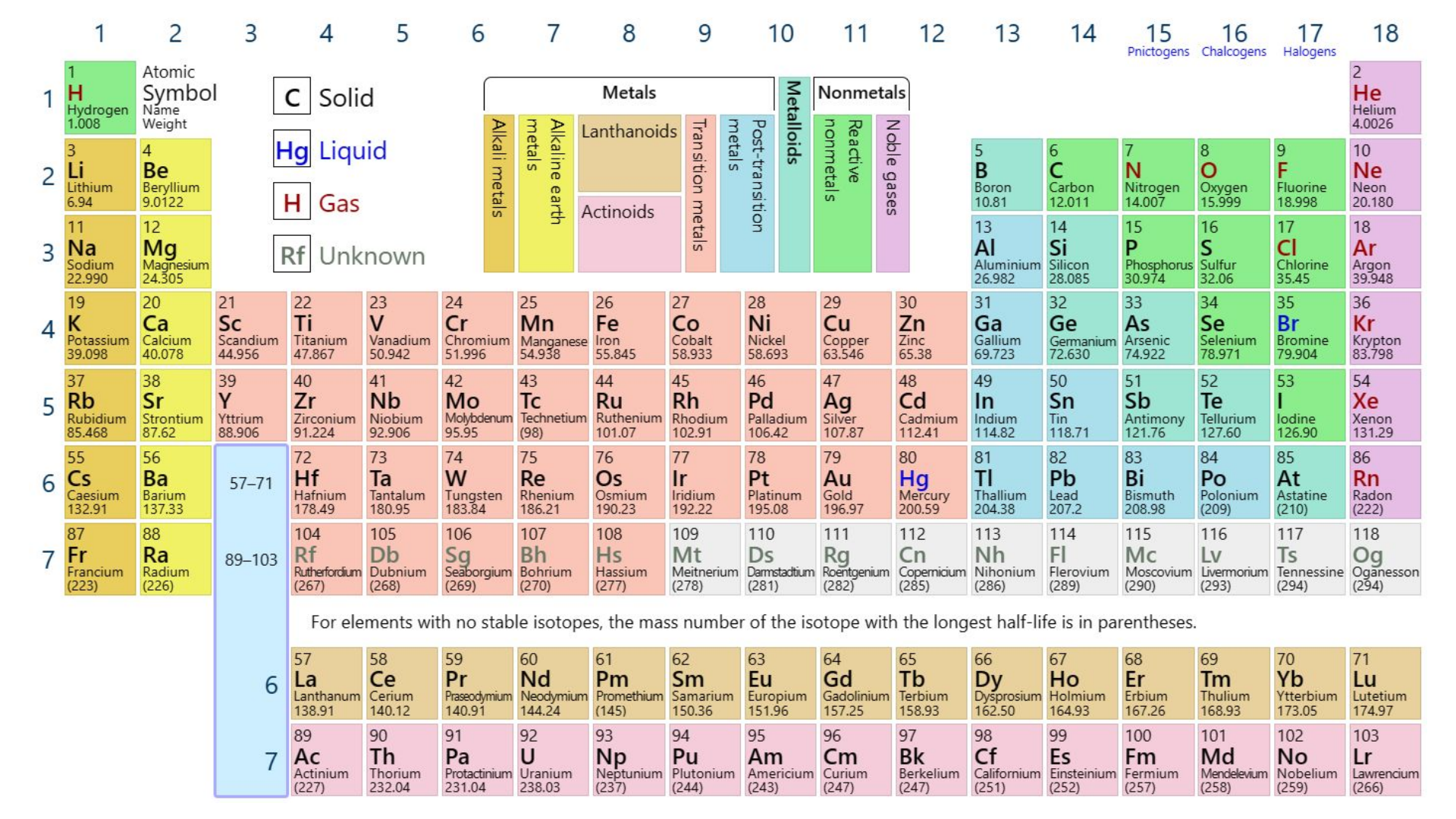
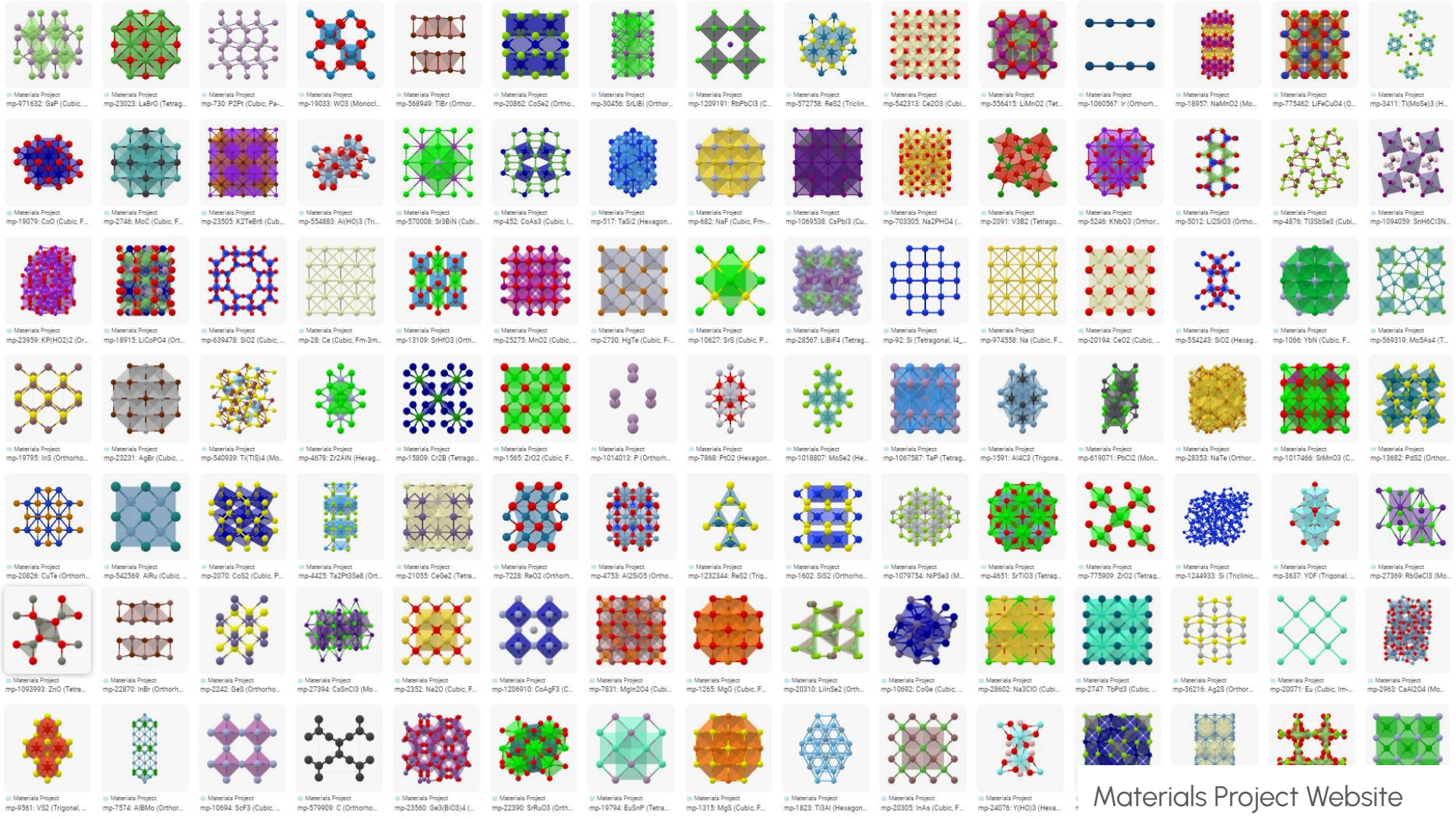





1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18
Pnictogens
Chalcogens
Halogens
Atomic
Symbol
Name
Weight
C Solid
Hg Liquid
H Gas
Rf Unknown
Metals
Alkali metals
Alkaline earth metals
Lanthanoids
Actinoids
Transition metals
Post-transition metals
Metalloids
Nonmetals
Reactive nonmetals
Noble gases
1 H Hydrogen 1.008
2 He Helium 4.0026
3 Li Lithium 6.94
4 Be Beryllium 9.0122
5 B Boron 10.81
6 C Carbon 12.011
7 N Nitrogen 14.007
8 O Oxygen 15.999
9 F Fluorine 18.998
10 Ne Neon 20.180
11 Na Sodium 22.990
12 Mg Magnesium 24.305
13 Al Aluminium 26.982
14 Si Silicon 28.085
15 P Phosphorus 30.974
16 S Sulfur 32.06
17 Cl Chlorine 35.45
18 Ar Argon 39.948
19 K Potassium 39.098
20 Ca Calcium 40.078
21 Sc Scandium 44.956
22 Ti Titanium 47.867
23 V Vanadium 50.942
24 Cr Chromium 51.996
25 Mn Manganese 54.938
26 Fe Iron 55.845
27 Co Cobalt 58.933
28 Ni Nickel 58.693
29 Cu Copper 63.546
30 Zn Zinc 65.38
31 Ga Gallium 69.723
32 Ge Germanium 72.630
33 As Arsenic 74.922
34 Se Selenium 78.971
35 Br Bromine 79.904
36 Kr Krypton 83.798
37 Rb Rubidium 85.468
38 Sr Strontium 87.62
39 Y Yttrium 88.906
40 Zr Zirconium 91.224
41 Nb Niobium 92.906
42 Mo Molybdenum 95.95
43 Tc Technetium (98)
44 Ru Ruthenium 101.07
45 Rh Rhodium 102.91
46 Pd Palladium 106.42
47 Ag Silver 107.87
48 Cd Cadmium 112.41
49 In Indium 114.82
50 Sn Tin 118.71
51 Sb Antimony 121.76
52 Te Tellurium 127.60
53 I Iodine 126.90
54 Xe Xenon 131.29
55 Cs Caesium 132.91
56 Ba Barium 137.33
57–71
72 Hf Hafnium 178.49
73 Ta Tantalum 180.95
74 W Tungsten 183.84
75 Re Rhenium 186.21
76 Os Osmium 190.23
77 Ir Iridium 192.22
78 Pt Platinum 195.08
79 Au Gold 196.97
80 Hg Mercury 200.59
81 Tl Thallium 204.38
82 Pb Lead 207.2
83 Bi Bismuth 208.98
84 Po Polonium (209)
85 At Astatine (210)
86 Rn Radon (222)
87 Fr Francium (223)
88 Ra Radium (226)
89–103
104 Rf Rutherfordium (267)
105 Db Dubnium (268)
106 Sg Seaborgium (269)
107 Bh Bohrium (270)
108 Hs Hassium (277)
109 Mt Meitnerium (278)
110 Ds Darmstadtium (281)
111 Rg Roentgenium (282)
112 Cn Copernicium (285)
113 Nh Nihonium (286)
114 Fl Flerovium (289)
115 Mc Moscovium (290)
116 Lv Livermorium (293)
117 Ts Tennessine (294)
118 Og Oganesson (294)
For elements with no stable isotopes, the mass number of the isotope with the longest half-life is in parentheses.
6
57 La Lanthanum 138.91
58 Ce Cerium 140.12
59 Pr Praseodymium 140.91
60 Nd Neodymium 144.24
61 Pm Promethium (145)
62 Sm Samarium 150.36
63 Eu Europium 151.96
64 Gd Gadolinium 157.25
65 Tb Terbium 158.93
66 Dy Dysprosium 162.50
67 Ho Holmium 164.93
68 Er Erbium 167.26
69 Tm Thulium 168.93
70 Yb Ytterbium 173.05
71 Lu Lutetium 174.97
7
89 Ac Actinium (227)
90 Th Thorium 232.04
91 Pa Protactinium 231.04
92 U Uranium 238.03
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 (259)
103 Lr Lawrencium (266)


Materials Project
mp-971632: GaP (Cubic, ...
mp-23023: LaBrO (Tetrag...
mp-730: P2Pt (Cubic, Pa-...
mp-19033: WO3 (Monocl...
mp-568949: TlBr (Orthor...
mp-20862: CoSe2 (Ortho...
mp-30456: SrLiBi (Orthor...
mp-1209191: RbPbCl3 (C...
mp-572758: ReS2 (Triclin...
mp-542313: Ce2O3 (Cubi...
mp-556415: LiMnO2 (Tet...
mp-1060567: Ir (Orthorh...
mp-18957: NaMnO2 (Mo...
mp-775462: LiFeCuO4 (O...
mp-3411: Ti(MoSe)3 (H...
mp-19079: CoO (Cubic, F...
mp-2746: MoC (Cubic, F...
mp-23505: K2TeBr6 (Cub...
mp-554883: Al(HO)3 (Tri...
mp-570008: Sr3BiN (Cubi...
mp-452: CoAs3 (Cubic, I...
mp-517: TaSi2 (Hexagon...
mp-682: NaF (Cubic, Fm-...
mp-1069538: CaPbI3 (Cu...
mp-703305: Na2PHO4 (...
mp-2091: V3B2 (Tetrago...
mp-5246: KNbO3 (Orthor...
mp-5012: Li2SiO3 (Ortho...
mp-4876: Ti3SbSe3 (Cubi...
mp-1094059: SnH6Cl3N...
mp-23959: KP(HO2)2 (Or...
mp-18915: LiCoPO4 (Ort...
mp-639478: SiO2 (Cubic, ...
mp-28: Ce (Cubic, Fm-3m...
mp-13109: SrHfO3 (Orth...
mp-25275: MnO2 (Cubic, ...
mp-2730: HgTe (Cubic, F-...
mp-10627: SrS (Cubic, P...
mp-28567: LiBiF4 (Tetrag...
mp-92: Si (Tetragonal, I4_...
mp-974558: Na (Cubic, F...
mp-20194: CeO2 (Cubic, ...
mp-554243: SiO2 (Hexag...
mp-1066: YbN (Cubic, F...
mp-569319: MoSbs4 (T...
mp-19795: InS (Orthorho...
mp-23231: AgBr (Cubic, ...
mp-540939: Ti(TlS)4 (Mo...
mp-4678: Zr2AlN (Hexag...
mp-13809: Cr2B (Tetrago...
mp-1565: ZrO2 (Cubic, F...
mp-1014013: P (Orthorh...
mp-7868: PtO2 (Hexagon...
mp-1018807: MoSe2 (He...
mp-1067587: TaP (Tetrag...
mp-1591: Al4C3 (Trigona...
mp-619071: PbCl2 (Mon...
mp-28353: NaTe (Orthor...
mp-1017466: SrMn03 (C...
mp-13682: PdS2 (Orthor...
mp-20826: CuTe (Orthorh...
mp-542569: AlRu (Cubic, ...
mp-2070: CoS2 (Cubic, P...
mp-4425: Ta2Pt3Se8 (Ort...
mp-21055: CeGe2 (Tetra...
mp-7228: ReO2 (Orthorh...
mp-4753: Al2SiO5 (Ortho...
mp-1232344: ReS2 (Triq...
mp-1602: SiS2 (Orthorho...
mp-1079754: NiPSe3 (M...
mp-4651: SrTiO3 (Tetrag...
mp-775909: ZrO2 (Tetrag...
mp-1244933: Si (Triclinic,...
mp-3637: YOF (Trigonal, ...
mp-27369: RbGeCl3 (Mo...
mp-1093993: ZnO (Tetra...
mp-22870: InBr (Orthorh...
mp-2242: GeS (Orthorho...
mp-27394: CsSnCl3 (Mo...
mp-2352: Na2O (Cubic, F...
mp-1206910: CoAgF3 (C...
mp-7831: MgIn2O4 (Cubi...
mp-1265: MgO (Cubic, F...
mp-20310: LiInSe2 (Orth...
mp-10692: CoGe (Cubic, ...
mp-28602: Na3ClO (Cubi...
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mp-36216: Ag2S (Orthor...
mp-20071: Eu (Cubic, Im-...
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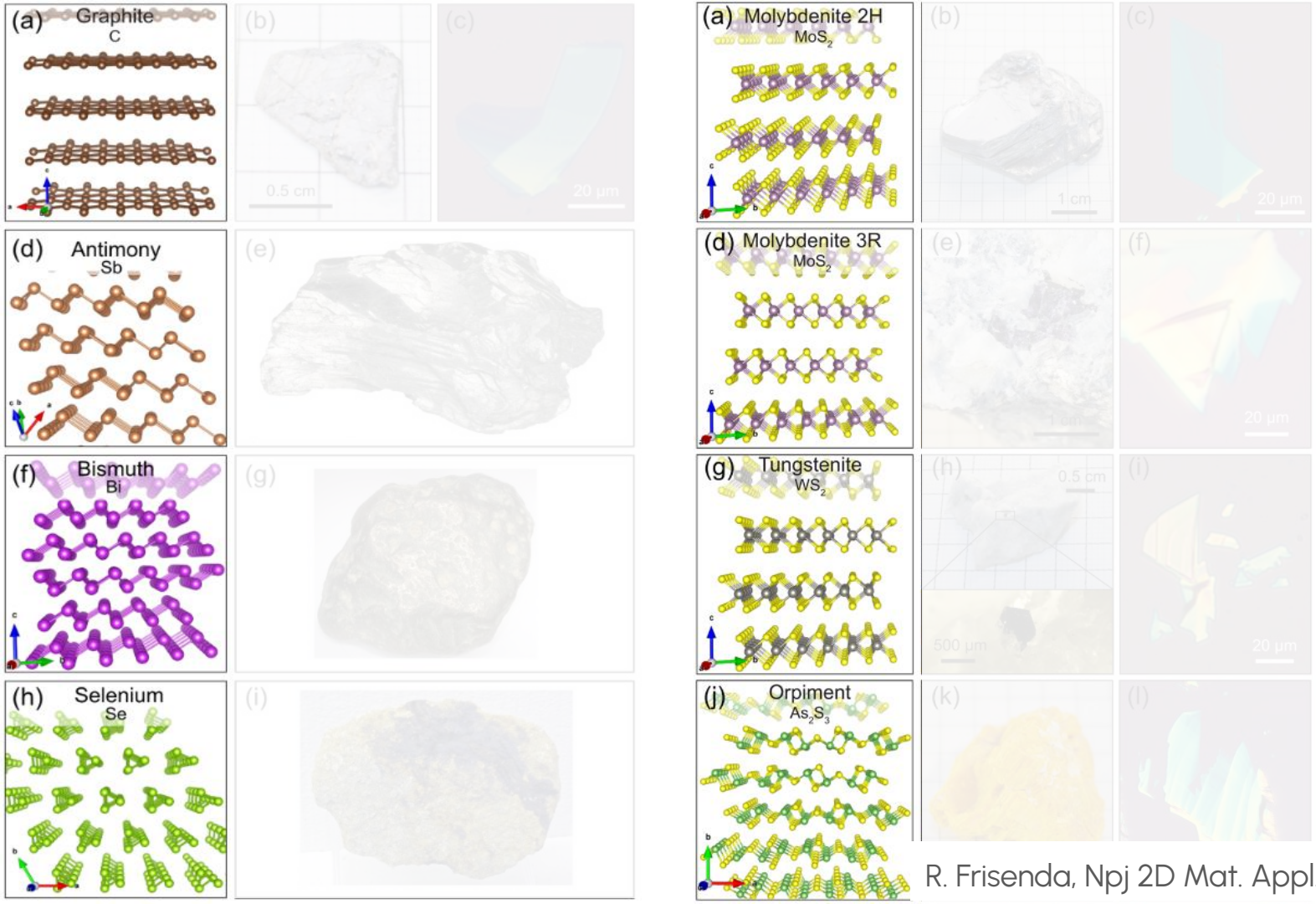
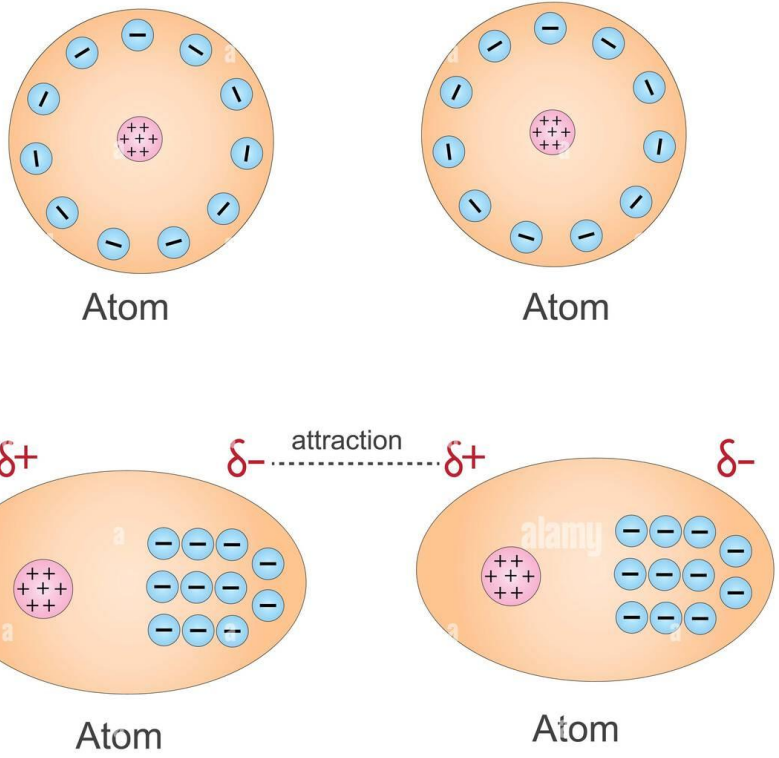
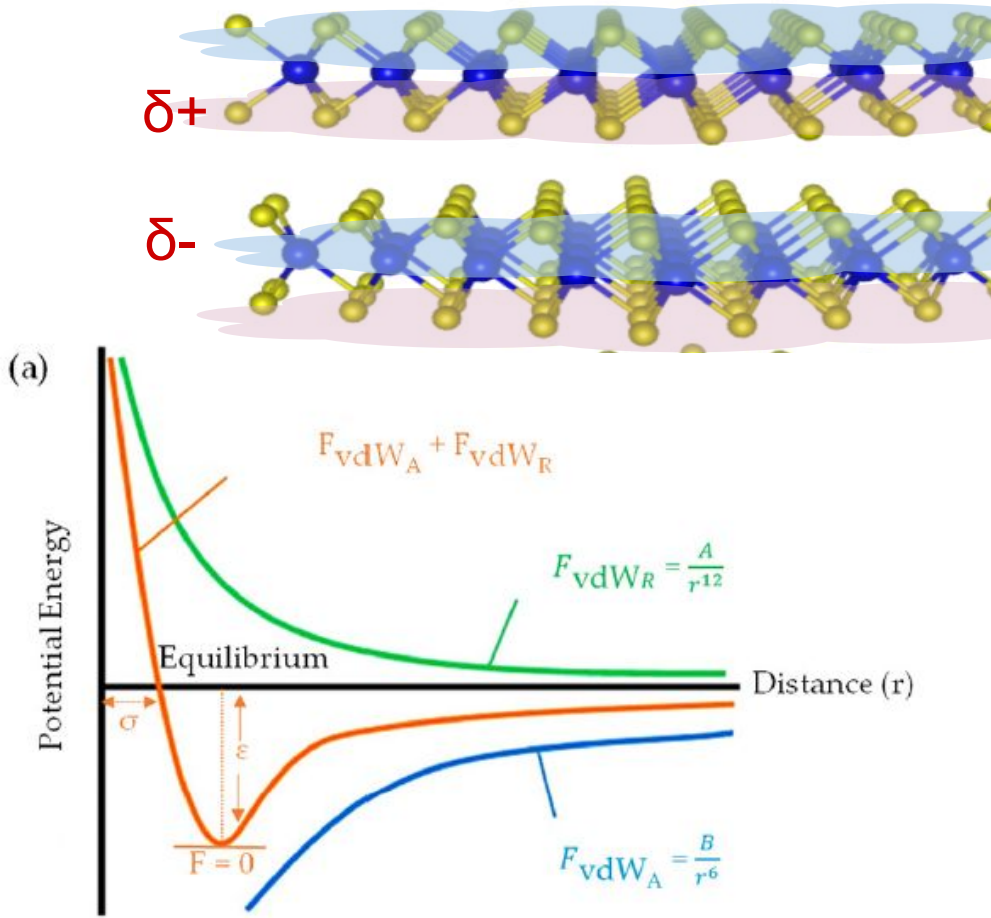
mp-9561: VS2 (Trigonal, ...
mp-7574: AlBMo (Orthor...
mp-10694: ScF3 (Cubic, ...
mp-579909: C (Orthorho...
mp-23560: Ge3(BiO3)4 (...
mp-22390: SrRuO3 (Orth...
mp-19794: EuSnP (Tetra...
mp-1315: MgS (Cubic, F...
mp-1823: TiSAl (Hexagon...
mp-20305: InAs (Cubic, F...
mp-24076: Y(HO)3 (Hexa...
Materials Project Website



R. Frisenda, Npj 2D Mat. Appl., 38, 2020

Van der Waals interactions





https://www.alamy.com/

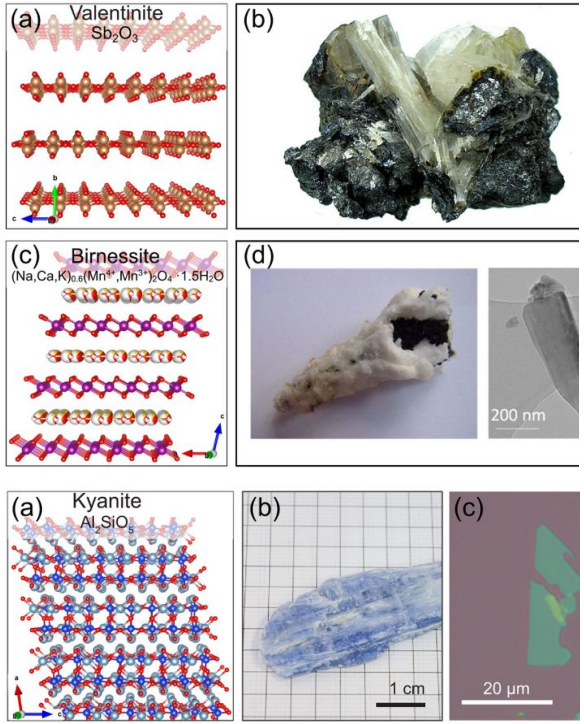
A. Brakat and H. Zhu, Nanomaterials, 13, 2399, 2023.

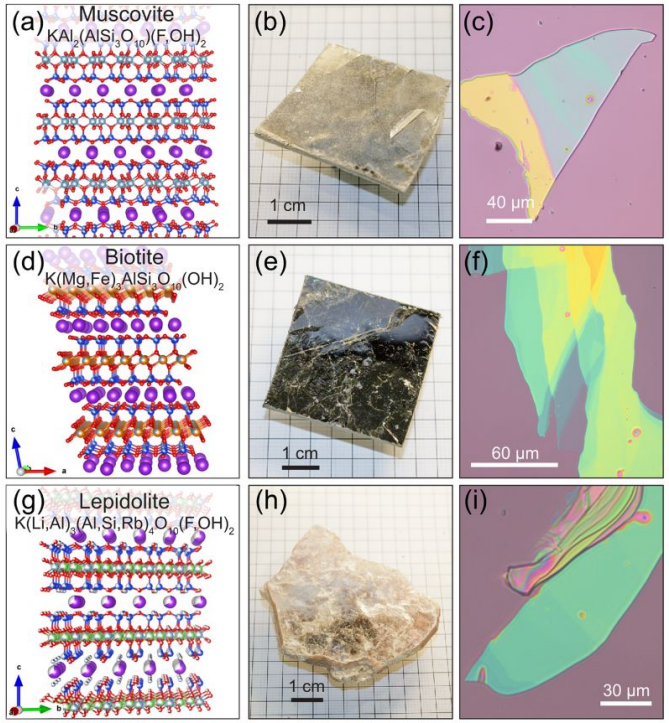
PERSPECTIVE OPEN

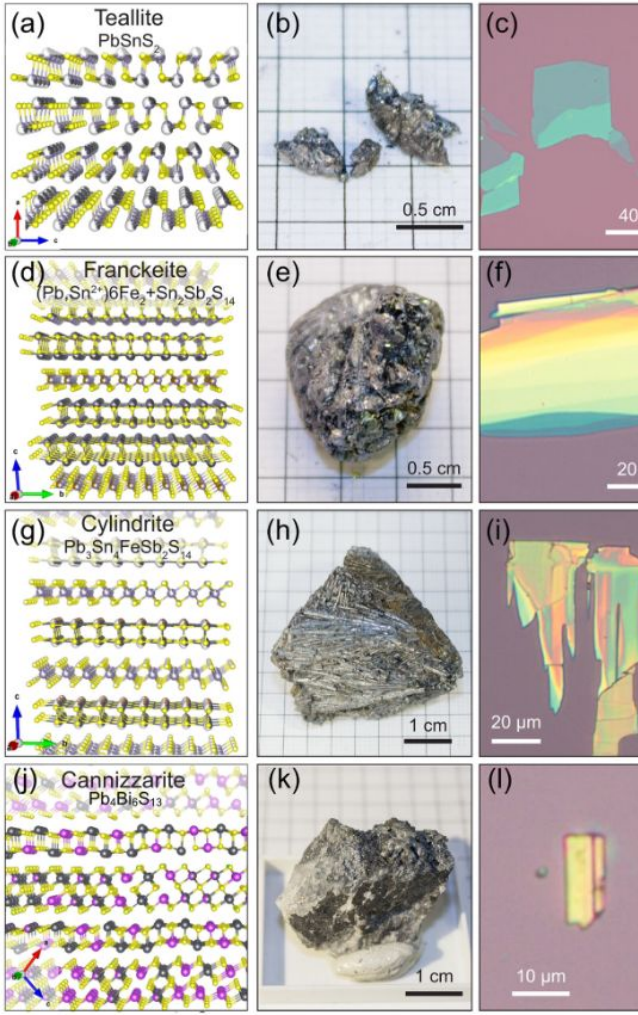
Naturally occurring van der Waals materials

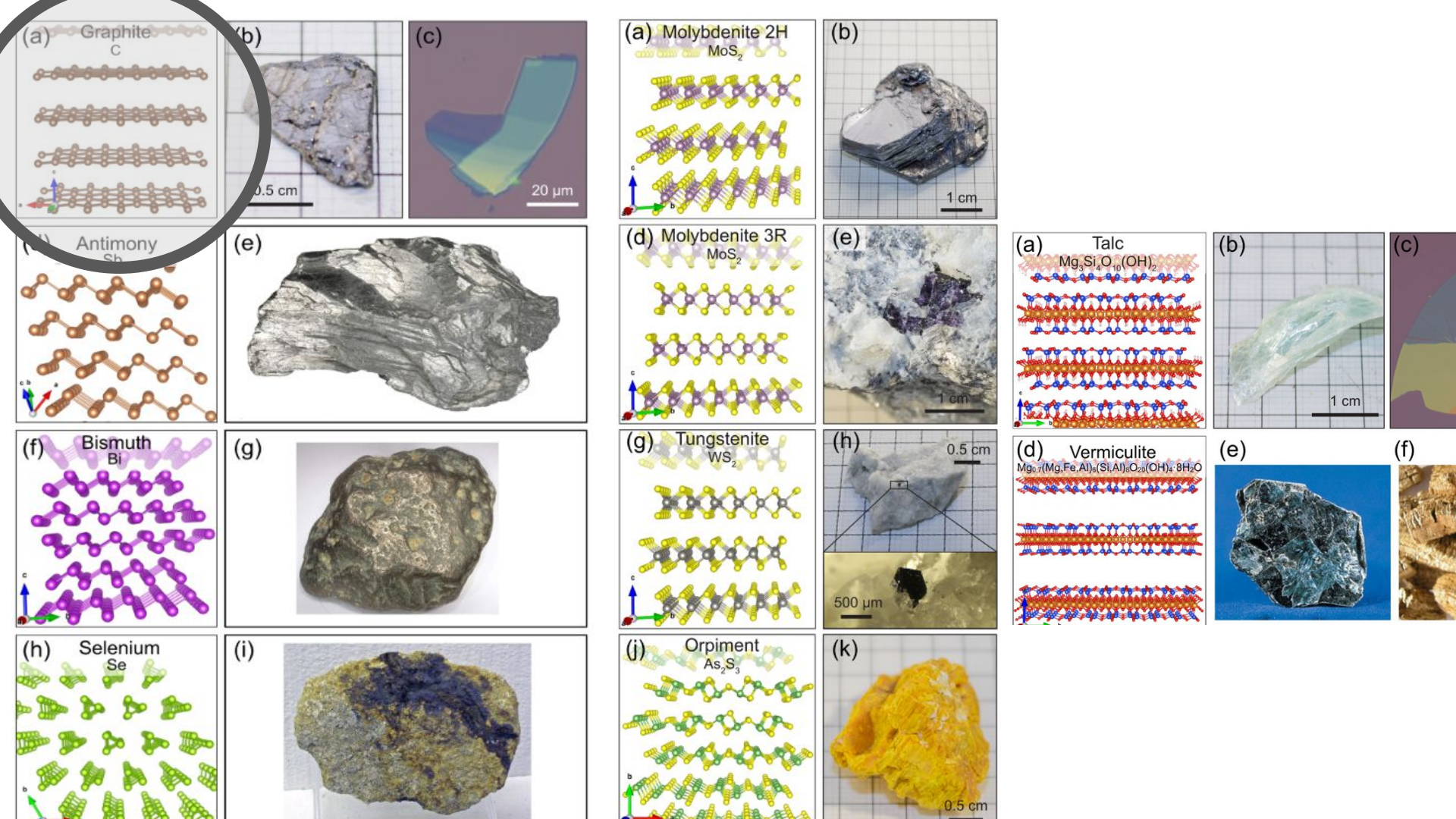
Riccardo Frisenda[1], Yue Niu[2], Patricia Gant[1], Manuel Muñoz[3] and Andres Castellanos-Gomez[1]✉

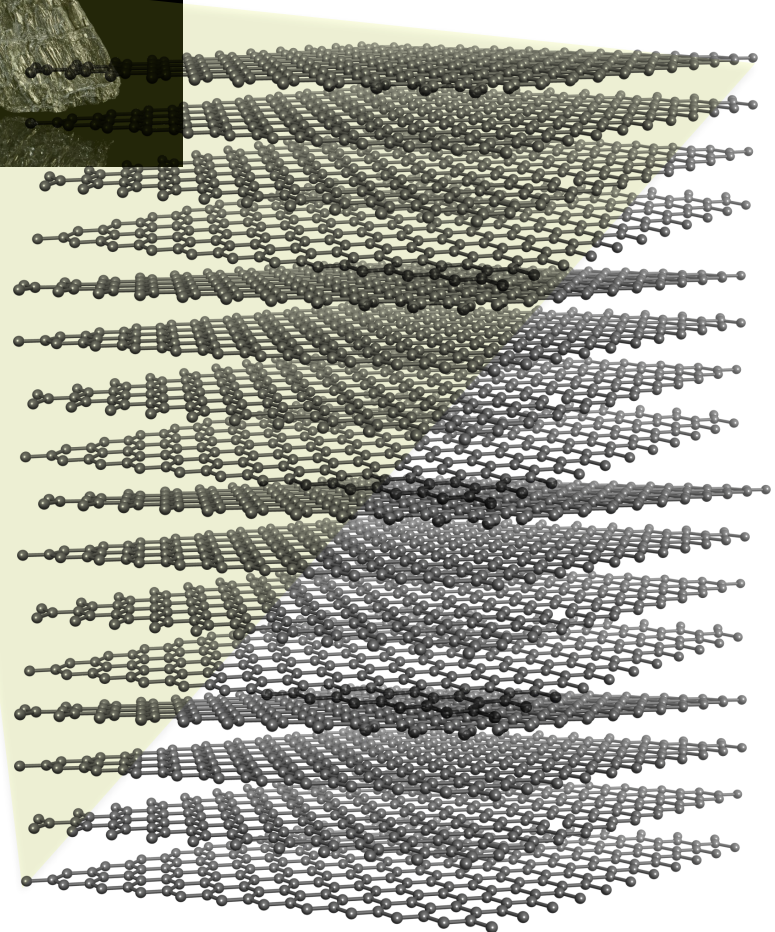
The exfoliation of two naturally occurring van der Waals minerals, graphite and molybdenite, arouse

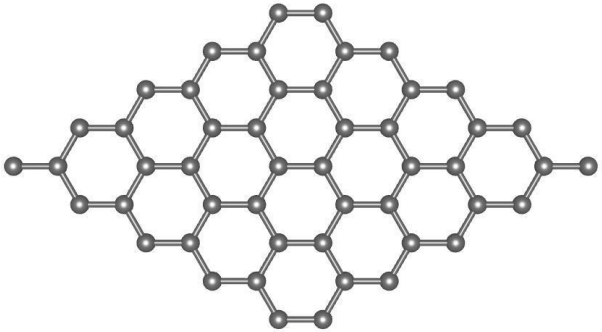


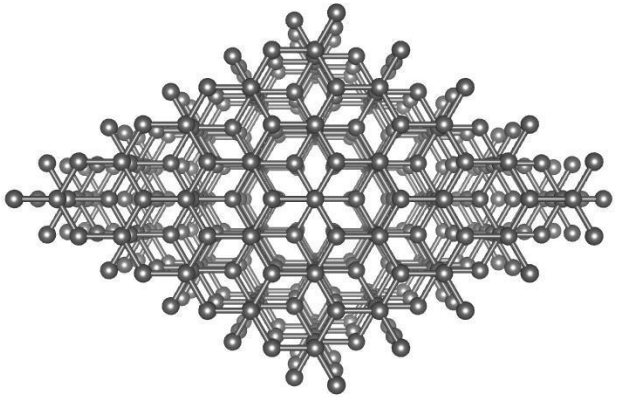




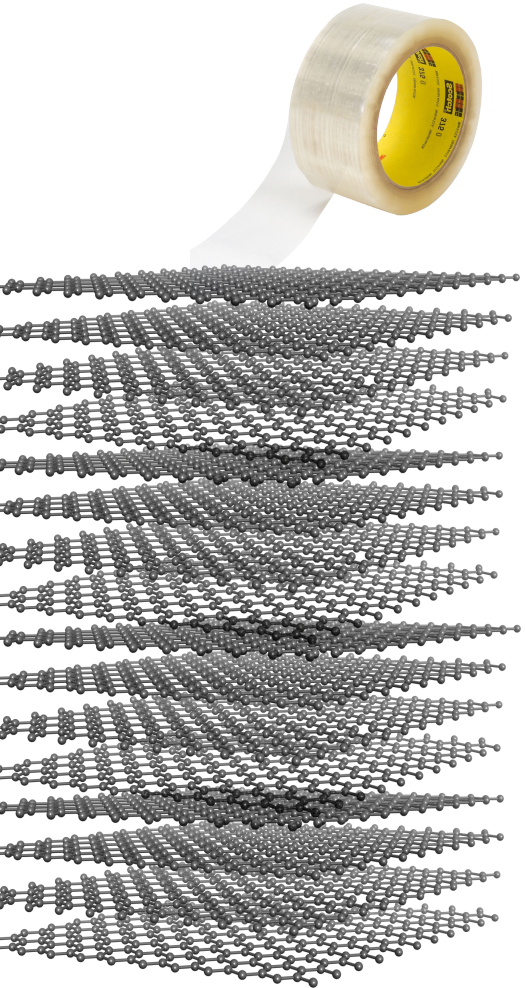

(a) Graphite
C
(b)
0.5 cm
(c)
20 μm
(a) Molybdenite 2H
MoS_2
(b)
1 cm
(a) Talc
$Mg_3Si_4O_{10}(OH)_2$
(b)
1 cm
(c)
(a) Antimony
Sb
(e)
(d) Molybdenite 3R
MoS_2
(e)
1 cm
(f) Bismuth
Bi
(g)
(g) Tungstenite
WS_2
(h)
0.5 cm
500 μm
(d) Vermiculite
$Mg_{0.7}(Mg,Fe,Al)_6(Si,Al)_8O_{20}(OH)_4 \cdot 8H_2O$
(e)
(f)
(h) Selenium
Se
(i)
(j) Orpiment
As_2S_3
(k)
0.5 cm

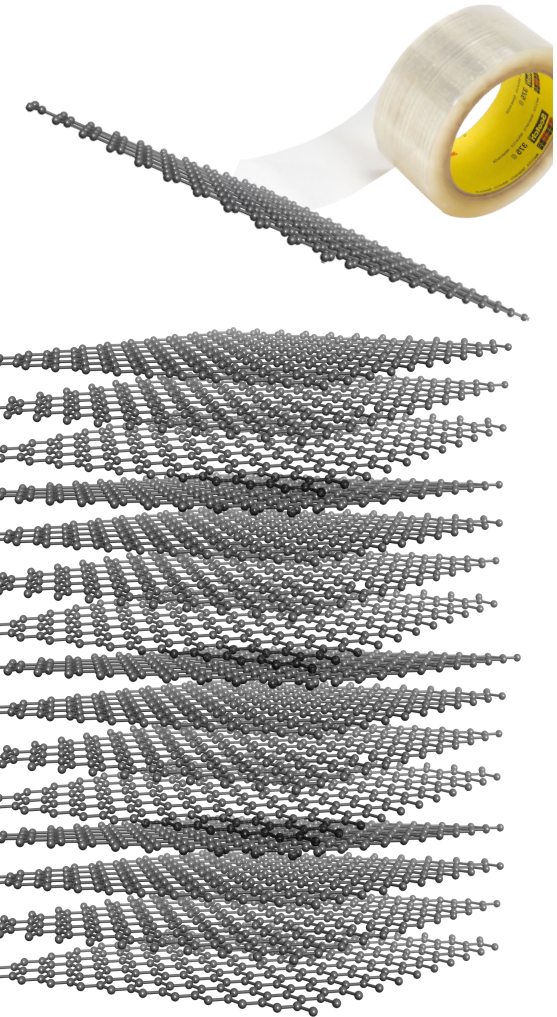






6
C
Carbon
12.011





Electric Field Effect in Atomically Thin Carbon Films

K. S. Novoselov,[1] A. K. Geim,[1]* S. V. Morozov,[2] D. Jiang,[1] Y. Zhang,[1] S. V. Dubonos,[2] I. V. Grigorieva,[1] A. A. Firsov[2]

We describe monocrystalline graphitic films, which are a few atoms thick but are nonetheless stable under ambient conditions, metallic, and of remarkably high quality. The films are found to be a two-dimensional semimetal with a tiny overlap

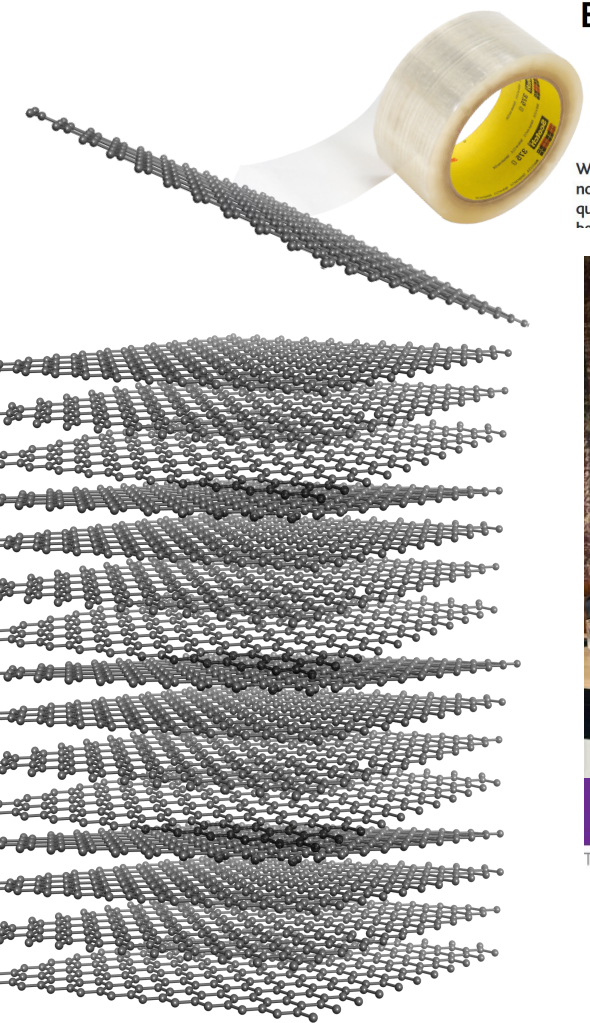
MANCHESTER 1824
The University of Manchester

Physics 2010

INTRODUCTION

The past decade has catalyzed the interest of the scientific community to study atomically thin materials (also known as two-dimensional (2D) materials). According to the Web of Science, the number of publications related to 2D materials have increased from ~1900 in 2004, when graphene was first isolated experimentally,[1] to ~49100 in 2021.[2] In that time, interest has expanded far beyond graphene. Other 2D

Yu Lei, et al. ACS Nanosci. Au, 2, 450, 2022.



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Physics 2010

Experimental observation of the quantum Hall effect and Berry's phase in graphene

Yuanbo Zhang[1], Yan-Wen Tan[1], Horst L. Stormer[1,2] & Philip Kim[1]

When electrons are confined in two-dimensional materials, quantum-mechanically enhanced transport phenomena such as the quantum Hall effect can be observed. Graphene, consisting of an isolated single atomic layer of graphite, is an ideal realization of such a two-dimensional system. However, its behaviour is expected to differ markedly from the well-studied case of quantum wells in conventional semiconductor interfaces. This difference arises from the unique electronic properties of graphene, which

electron-like and hole-like carriers tuned by the electric field effect[8,9,11]. However, the quantum Hall effect (QHE) was not observed in these samples, possibly as a result of their low mobility and/or the residual three-dimensional nature of the specimens.

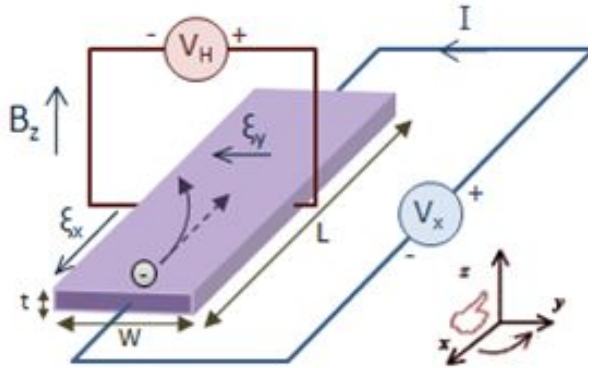
The high-mobility graphene samples used in our experiments were extracted from Kish graphite (Toshiba Ceramics) on degenerately doped Si wafers with a 300-nm SiO_2 coating layer, by using micromechanical manipulation similar to that described in ref. 8.

Yu Lei, et al. ACS Nanosci. Au, 2, 450, 2022.

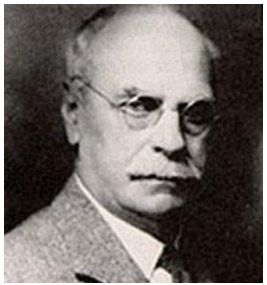
- ***Thinnest.*** At one atom thick, it's the thinnest material we can see.
- ***Lightest.*** One square meter of graphene weighs about 0.77 milligrams. For scale, one square meter of regular paper is 1000 times heavier than graphene and a single sheet of graphene big enough to cover a football field would weigh less than a gram.
- ***Strongest***. Graphene is stronger than steel and Kevlar, with a tensile strength of 150,000,000 psi.
- ***Stretchiest***. Graphene has an amazing ability to retain its initial size after strain. Graphene sheets suspended over silicone dioxide cavities had spring constants in the region of 1-5 N/m and a Young's modulus of 0.5 TPa.
- ***Best Conductor of Heat***. At room temperature, graphene's heat conductivity is (4.84±0.44) × 10^3 to (5.30 ±0.48) × 10^3 W·m−1·K−1.
- ***Best Conductor of Electricity***. In graphene, each carbon atom is connected to three other carbon atoms on a two-dimensional plane, which leaves one electron free for electronic conduction. Recent studies have shown electron mobility at values more than 15,000 cm2·V−1·s−1. Graphene moves electrons 10 times faster than silicon using less energy.
- ***Best Light Absorber***. Graphene can absorb 2.3% of white light, which is remarkable because of its extreme thinness. This means that, once optical intensity reaches saturation fluence, saturable absorption takes place, which makes it possible to achieve full-band mode locking.
- ***Most Renewable.*** Statistically speaking, carbon is the fourth most abundant element in the entire universe (by mass). Because of this abundance, graphene could well be a sustainable, ecologically friendly solution for an increasingly complex world.
- ***Most Exceptional.*** What most captures the imagination is that graphene is one simple material that by itself possesses all these astonishing qualities. No other material in the world is the thinnest, strongest, lightest, and stretchiest, and can conduct heat and electricity super-fast, all at the same time.

https://www.acsmaterial.com/graphene-facts

Hall Effect

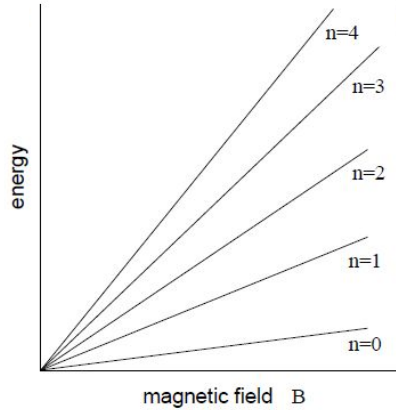


$$\mathbf{F} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B})$$



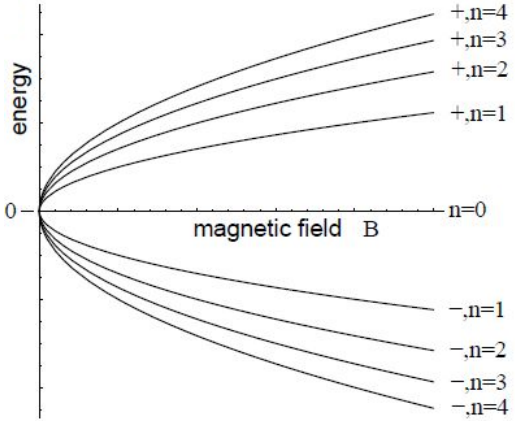
Edwin Herbert Hall
(1879)

Quantum Hall Effect



$$\epsilon_n = \hbar\omega_C(n + 1/2)$$
$$\propto B(n + 1/2)$$

Anomalous Quantum Hall Effect



$$\epsilon_{\lambda,n} = \lambda(\hbar v/l_B)\sqrt{2n}$$
$$\propto \lambda\sqrt{Bn}$$

Mark O. Goerbig, Quantum Hall Effects, 2009.

Intrinsic ripples in graphene

A. FASOLINO*, J. H. LOS AND M. I. KATSNELSON
Institute for Molecules and Materials, Radboud University Nijmegen, Toernooiveld 1, 6525ED Nijmegen, The Netherlands
*e-mail: a.fasolino@science.ru.nl

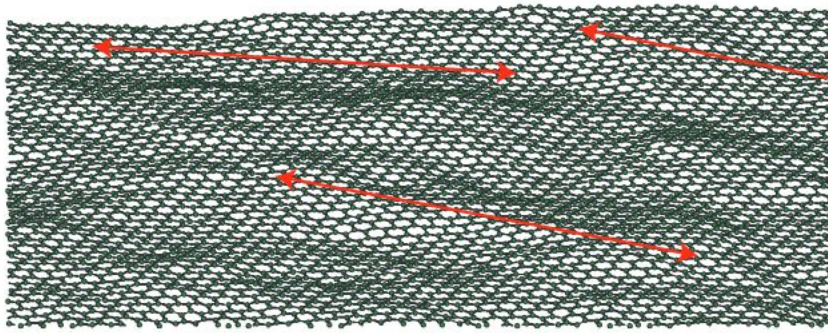


Figure 1 A representative configuration of the $N = 8{,}640$ sample a
The red arrows are ~80 Å long.

The stability of two-dimensional (2D) layers and is the subject of a long-standing theoretical debate to the so-called Mermin–Wagner theorem[1], long-wavelength fluctuations destroy the long-range order of 2D crystals. Similarly, 2D membranes embedded in a 3D space have a tendency to be crumpled[2]. These fluctuations can, however, be suppressed by anharmonic coupling between bending and stretching modes meaning that a 2D membrane can exist but will exhibit strong height fluctuations[2–4]. The discovery of

Two-dimensional atomic crystals

K. S. Novoselov*, D. Jiang*, F. Schedin*, T. J. Booth*, V. V. Khotkevich*, S. V. Morozov†, and A. K. Geim*‡

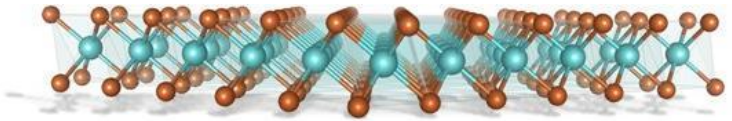
*Centre for Mesoscience and Nanotechnology and School of Physics and Astronomy, University of Manchester, Manchester M13 9PL, United Kingdom; and †Institute for Microelectronics Technology, Chernogolovka 142432, Russia

Edited by T. Maurice Rice, Swiss Federal Institute of Technology, Zurich, Switzerland, and approved June 7, 2005 (received for review April 6, 2005)

We report free-standing atomic crystals that are strictly 2D and can be viewed as individual atomic planes pulled out of bulk crystals or as unrolled single-wall nanotubes. By using micromechanical cleavage, we have prepared and studied a variety of 2D crystals including single layers of boron nitride, graphite, several dichalcogenides, and complex oxides. These atomically thin sheets (essentially gigantic 2D molecules unprotected from the immediate environment) are stable under ambient conditions, exhibit high crystal quality, and are continuous on a macroscopic scale.

wafer (Fig. 1*d*), because even a monolayer adds up sufficie
to the optical path of reflected light so that the interference c
changes with respect to the one of an empty substrate (ph
contrast). The whole procedure takes literally half an hou
implement and identify probable 2D crystallites. Their furt
analysis was done by atomic force microscopy (AFM), for wl
single-layer crystals were selected as those exhibiting an ap
ent (12) thickness of approximately the interlayer distance in
corresponding 3D crystals.

Transition Metal Dichalcogenides (TMDCs)



MX_2

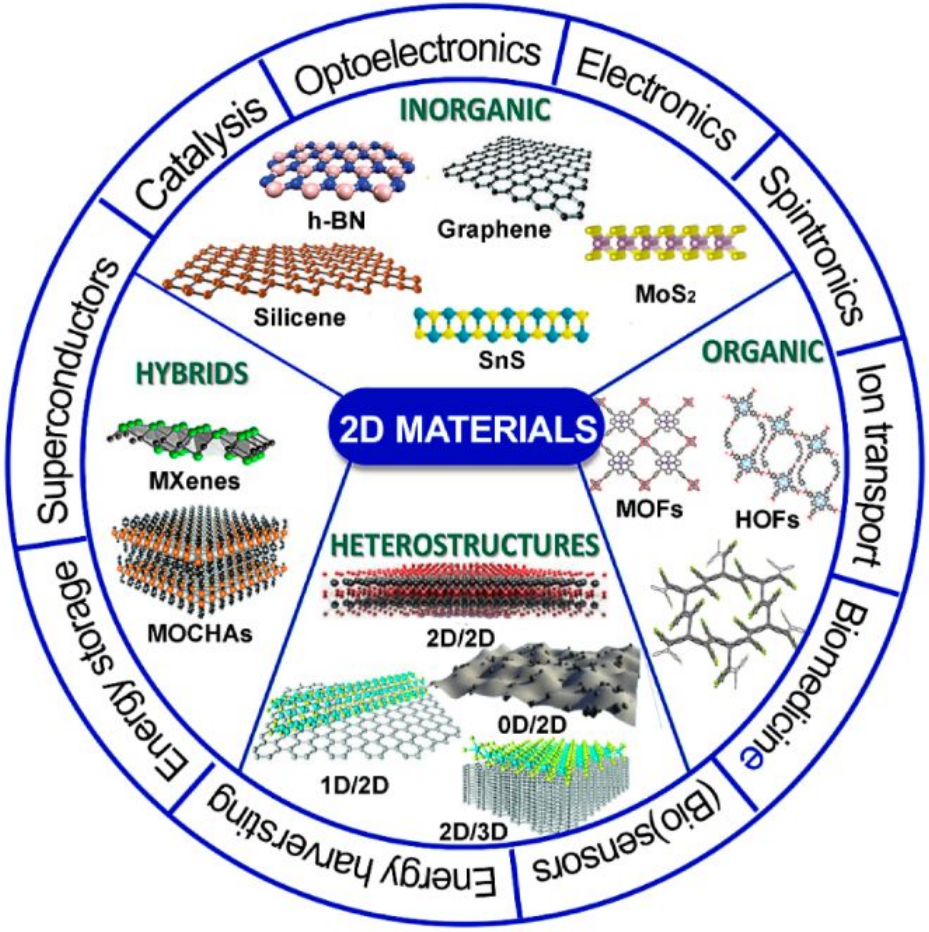
Materiais ~~bidimensionais~~ atomicamente finos

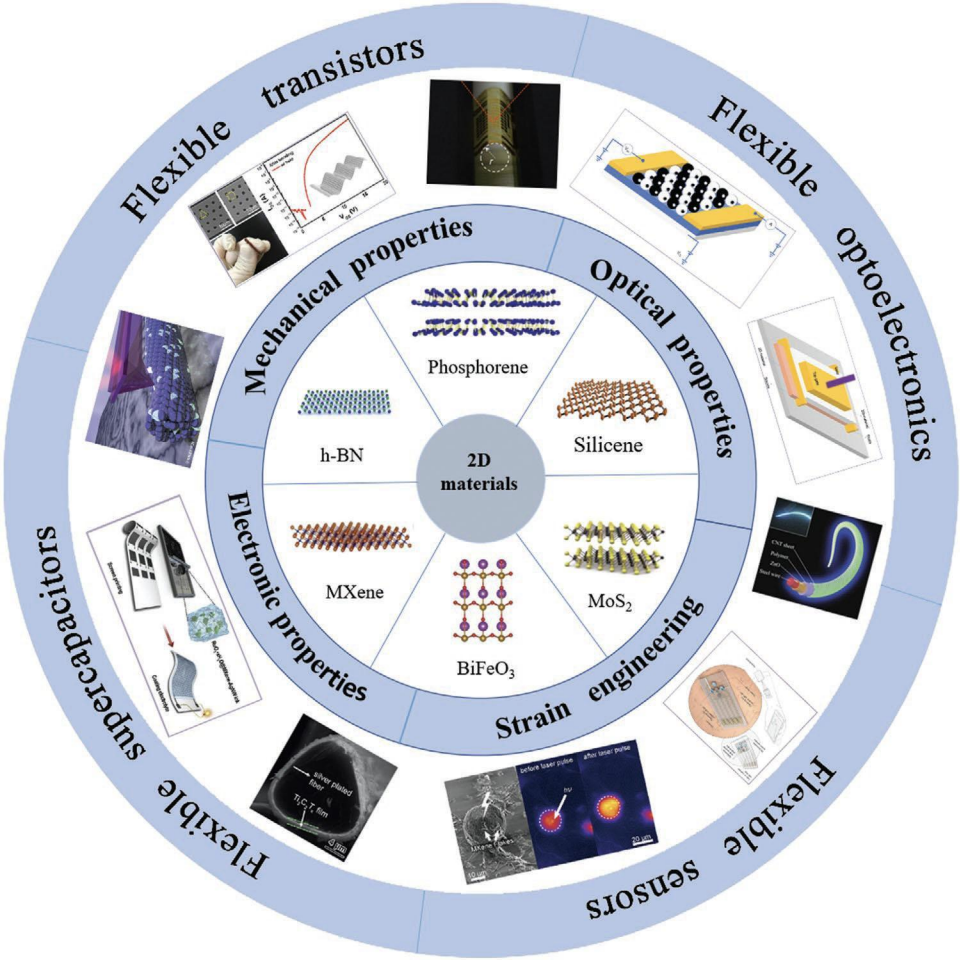
O que são?

Cristais com um ou poucos átomos de espessura

Interações eletrônicas no plano são muito mais fortes do que aquelas na direção perpendicular ao plano.

Para que servem?





D. Scarano, *Materials, 14*(23), 7108, 2021.

https://www.nanowerk.com/spotlight/spotid=60554.php

Quantum Information

2D materials for quantum information science

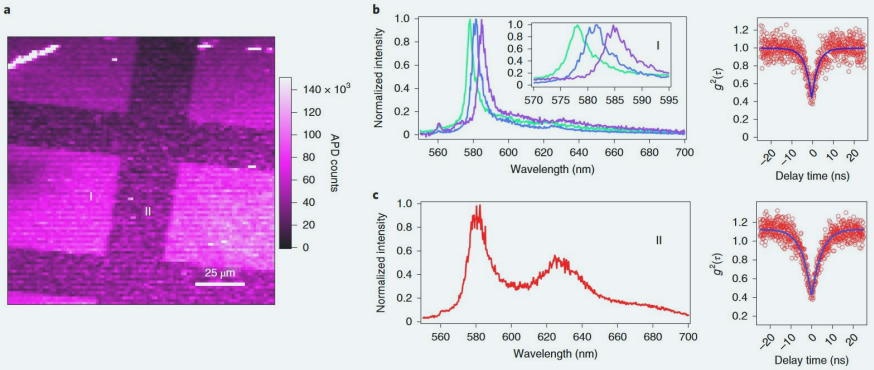
*Xiaolong Liu[1] and Mark C. Hersam[1,2,3,4]**

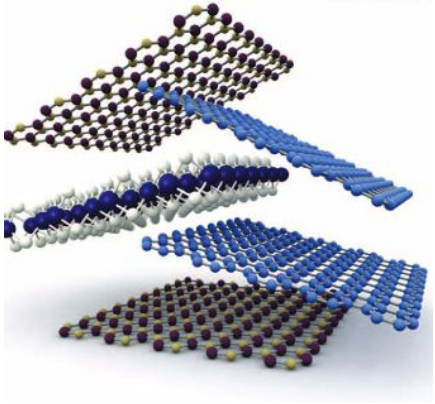
Abstract | The transformation of digital computers from bulky machines to portable sy
been enabled by new materials and advanced processing technologies that allow ultr

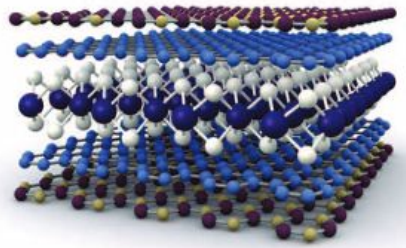
Identifying carbon as the source of visible single-photon emission from hexagonal boron nitride

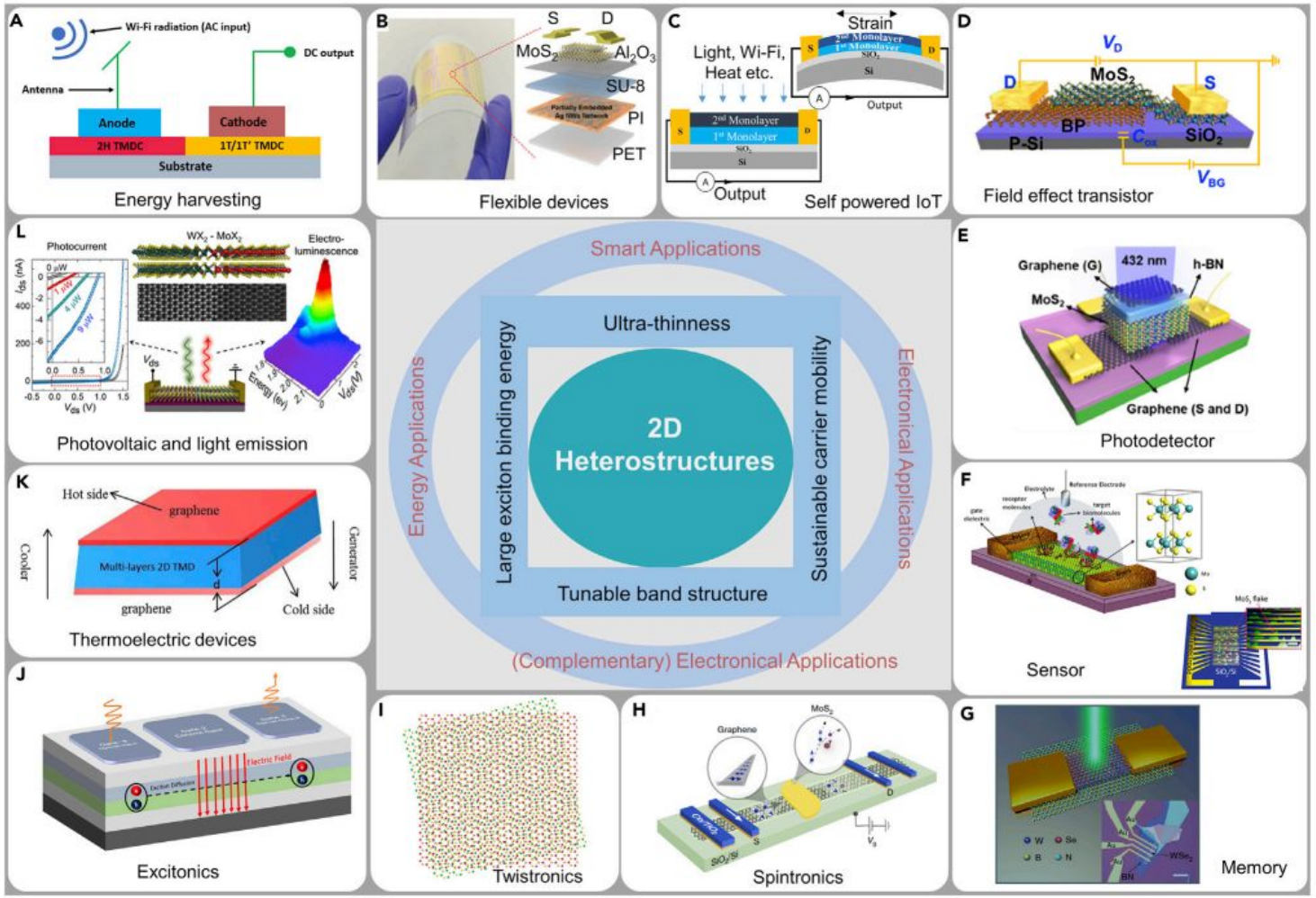
Noah Mendelson[1], Dipankar Chugh[2], Jeffrey R. Reimers[1,3], Tin S. Cheng[4], Andreas Gottscholl[5], Hu Long[6,7,8], Christopher J. Mellor[4], Alex Zettl[6,7,8], Vladimir Dyakonov[5], Peter H. Beton[4], Sergei V. Novikov[4], Chennupati Jagadish[2,9], Hark Hoe Tan[2,9], Michael J. Ford[1], Milos Toth[1,10], Carlo Bradac[1,11] and Igor Aharonovich[1,10] ✉

Single-photon emitters (SPEs) in hexagonal boron nitride (hBN) have garnered increasing attention over the last few years due to their superior optical properties. However, despite the vast range of experimental results and theoretical calculations, the





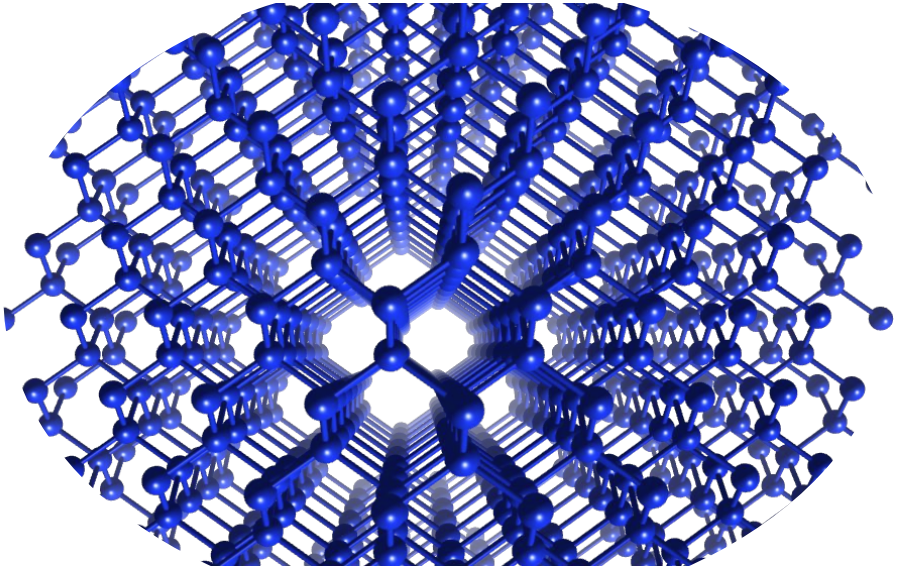


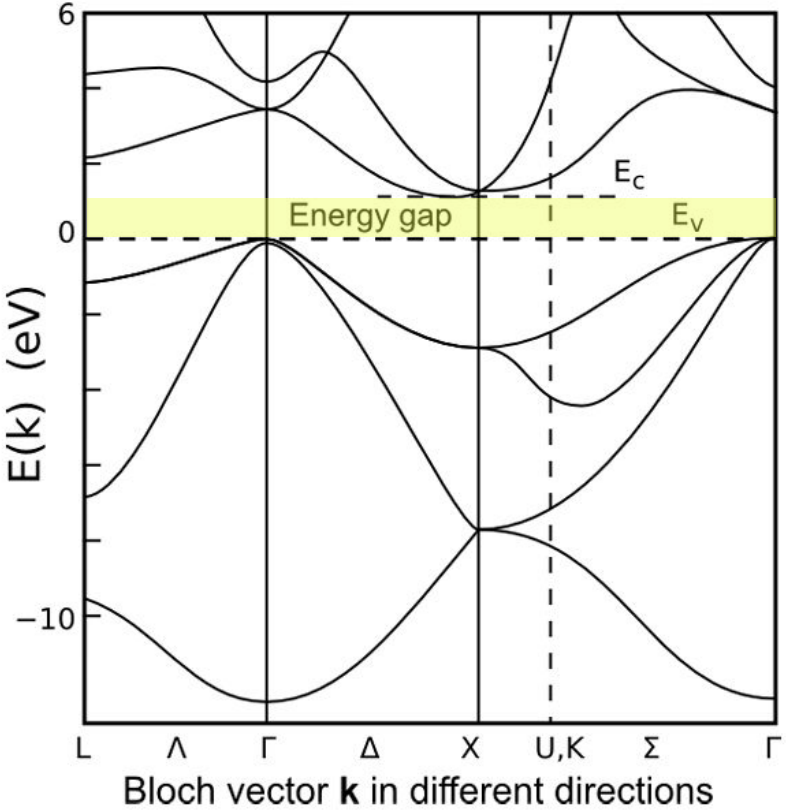


K. S. Novoselov, Science, 353, 2016

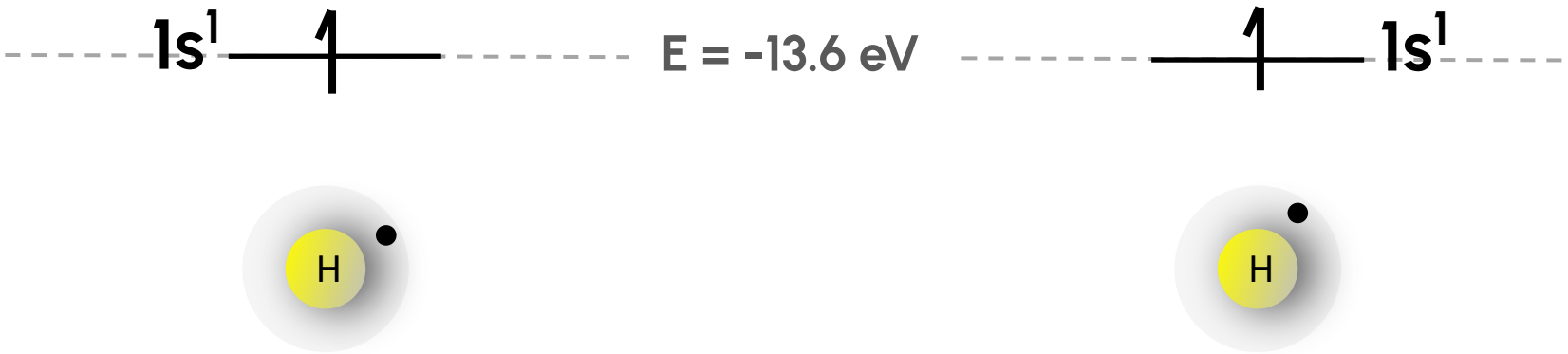
S. K. Chakraborty, iScience 25, 103942, 2022

Electronic Band Structure

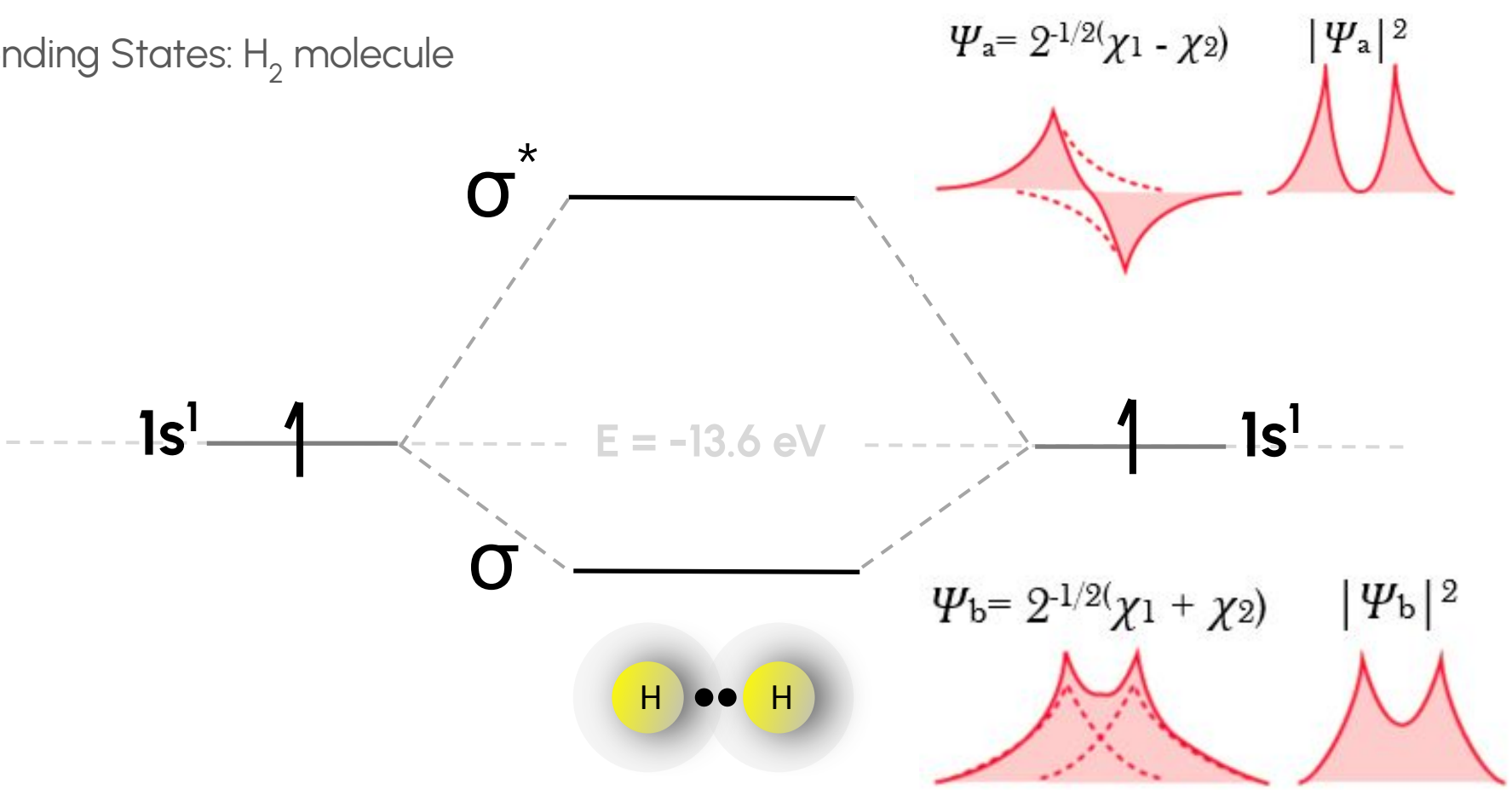




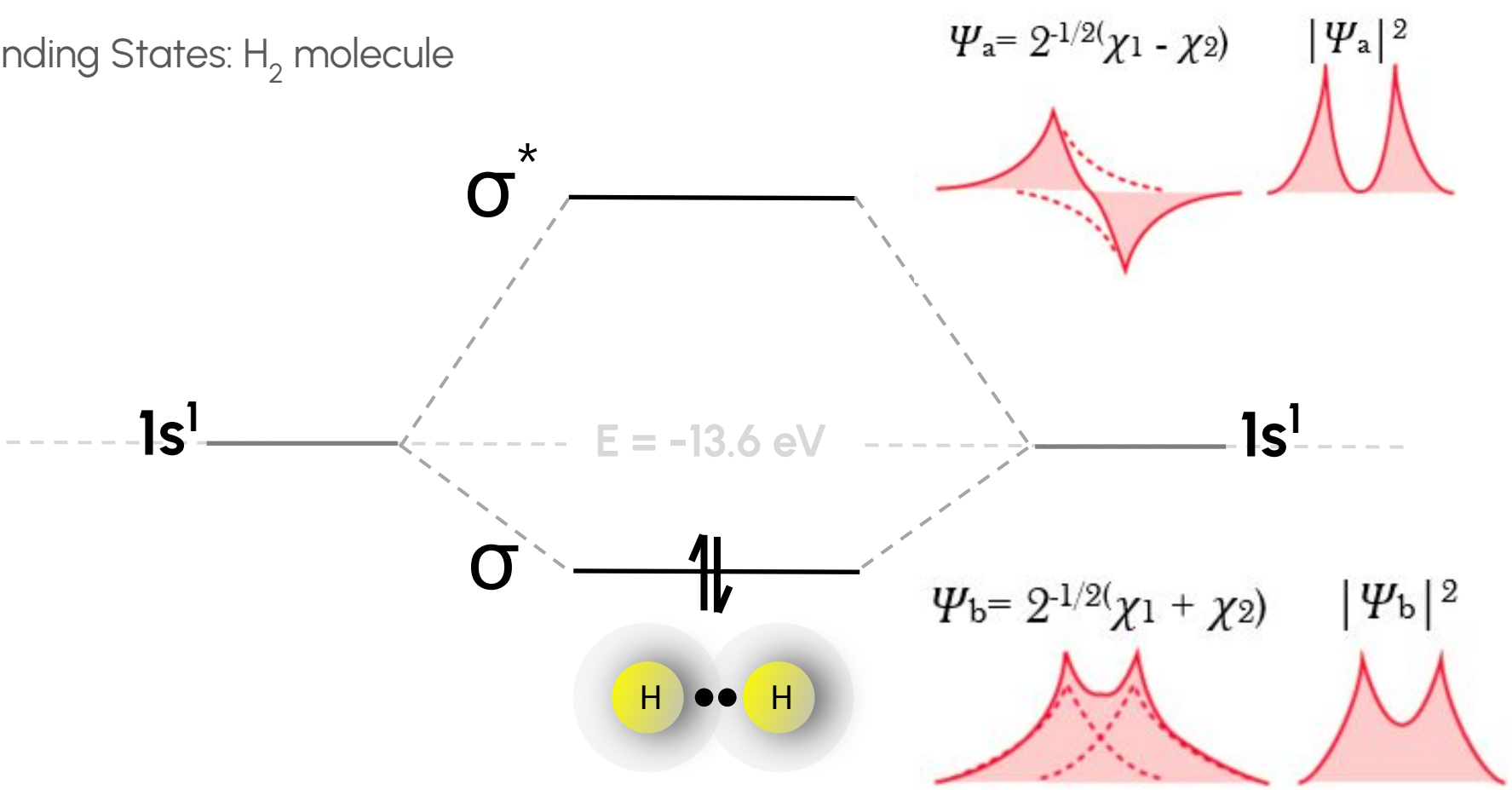
Bonding States: H_2 molecule



Bonding States: H_2 molecule

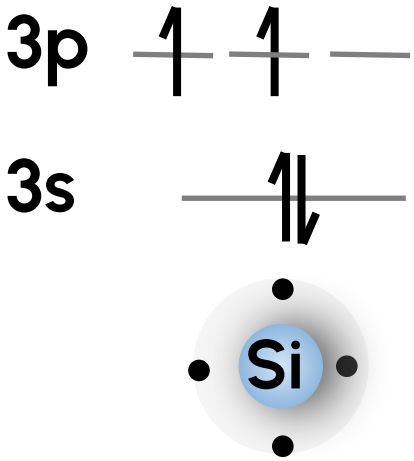


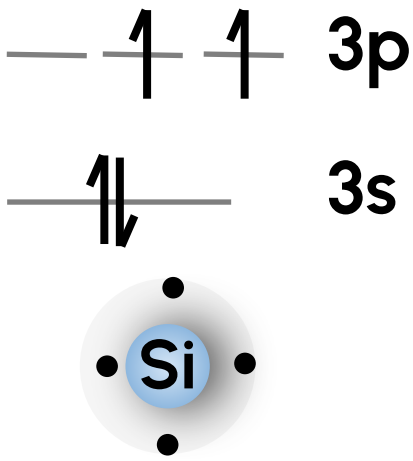
Bonding States: H_2 molecule



Electronic Band Structure: Si crystal

Valência: $3s^2\ 3p^2$





Electronic Band Structure: Si crystal

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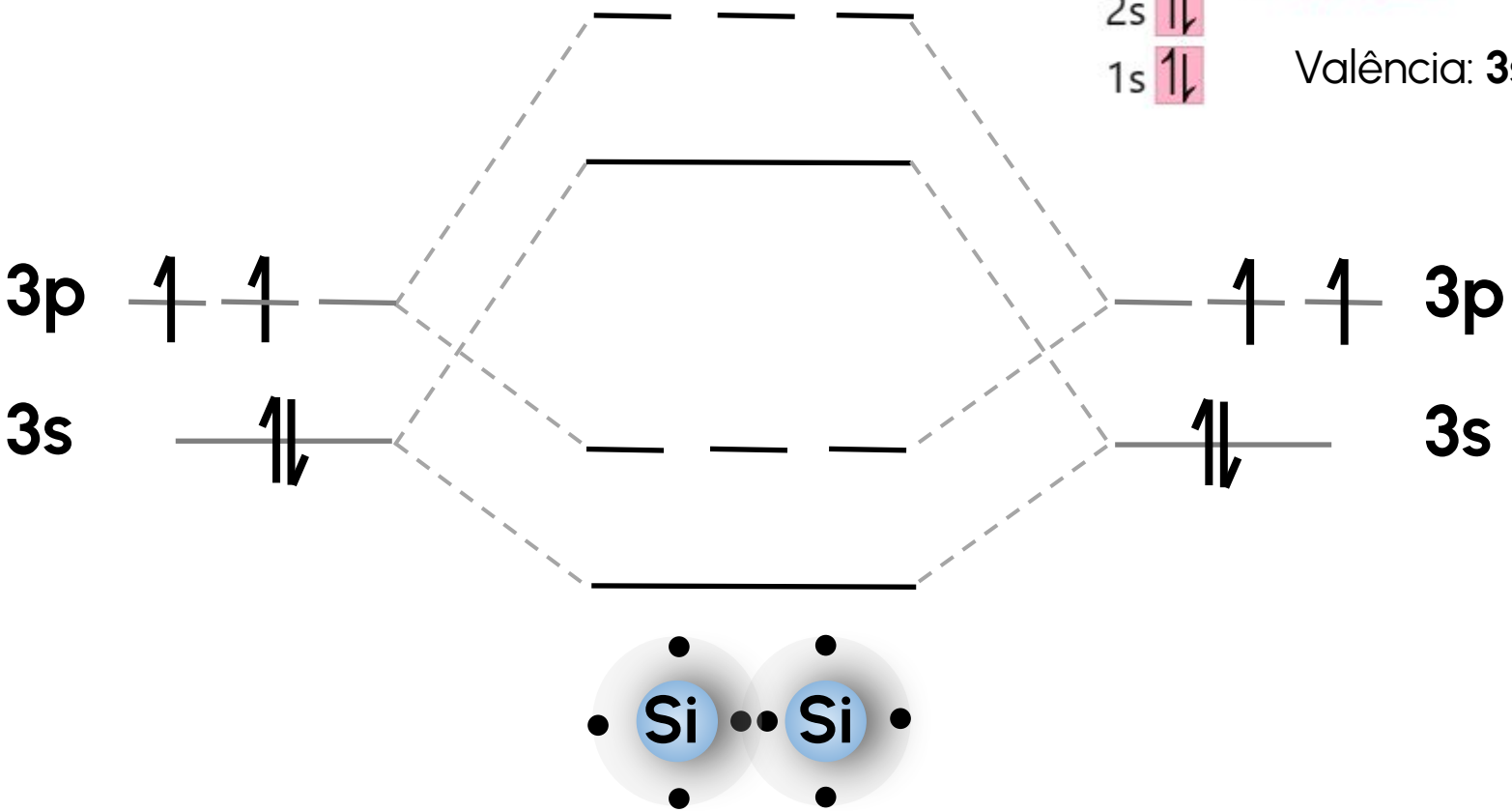

Electronic Band Structure: Si crystal

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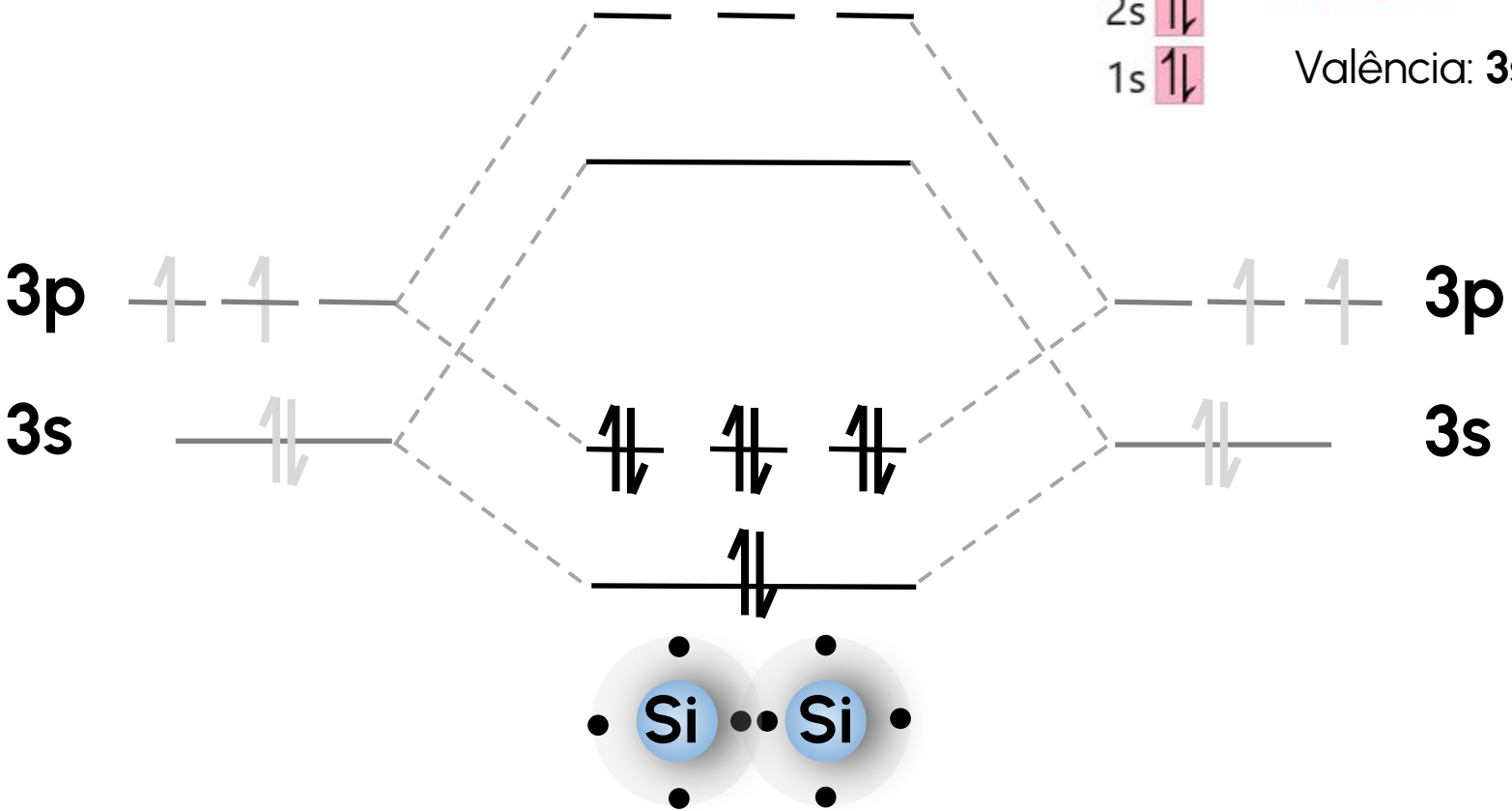
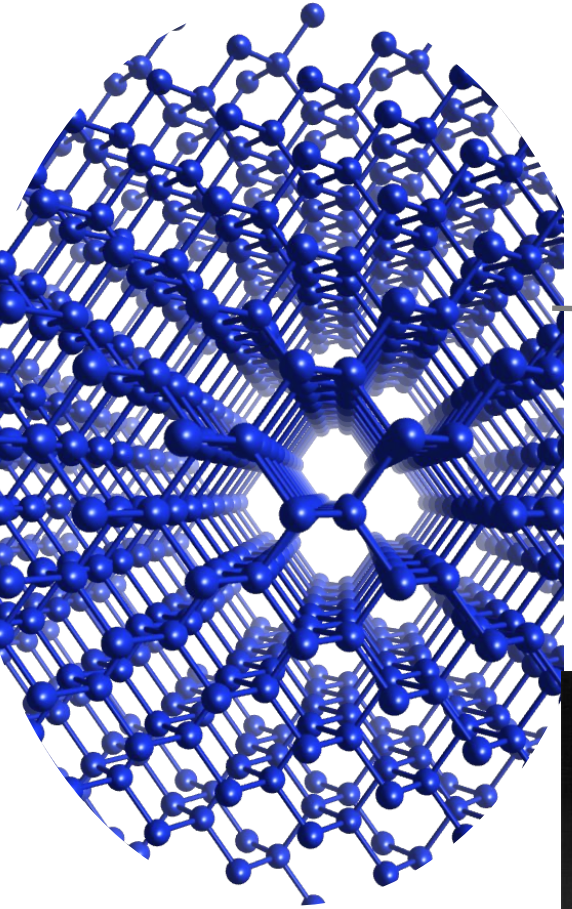
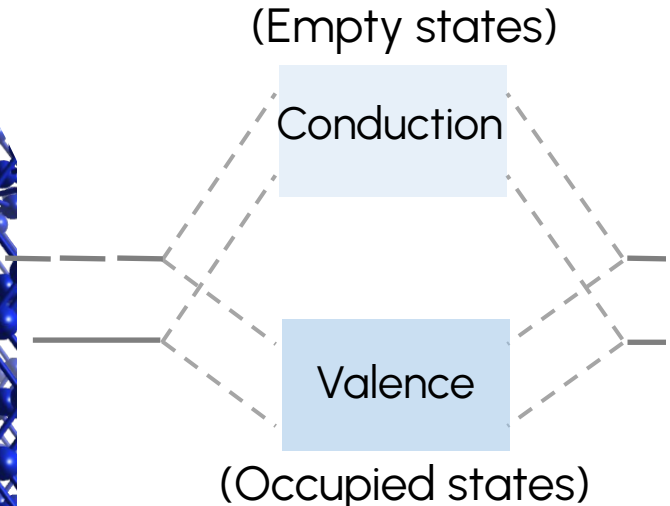
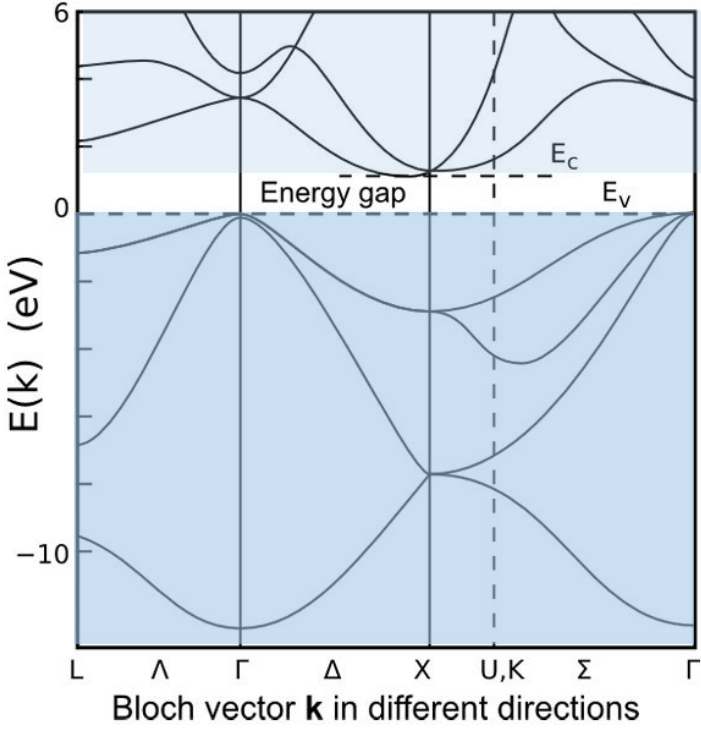


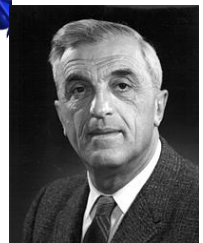
Electronic Band Structure: Si crystal

If we have **a lot of** atoms? (~ 10^{23})









Felix Bloch
(1905-1983)

Bloch's Theorem

$$\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u(\mathbf{r})$$

Andreas Wacker Notes (2018)

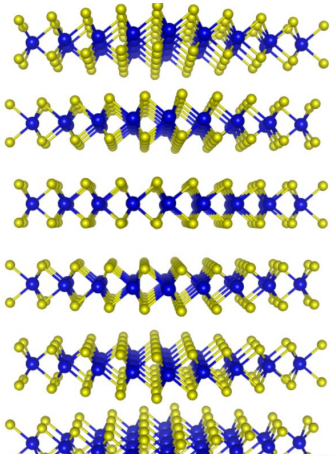
Band Gap Tuning: TMDCs

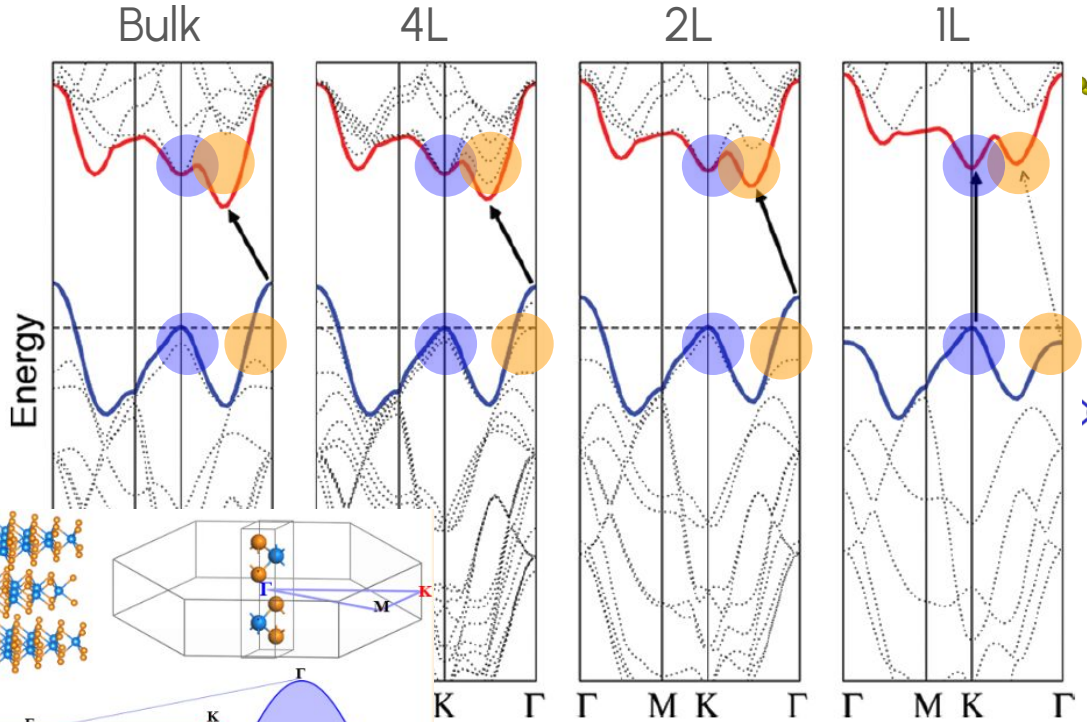
TX_2

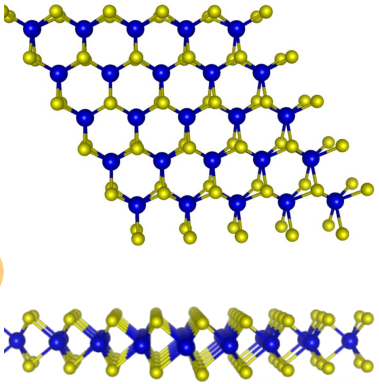
MoS_2

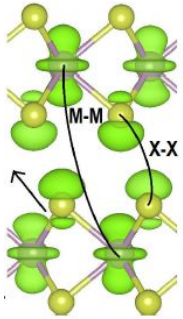
Mo-d

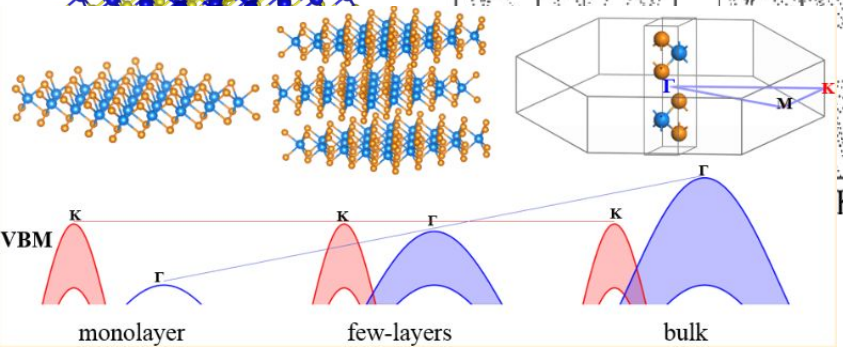
Mo-d + **S**-p_z





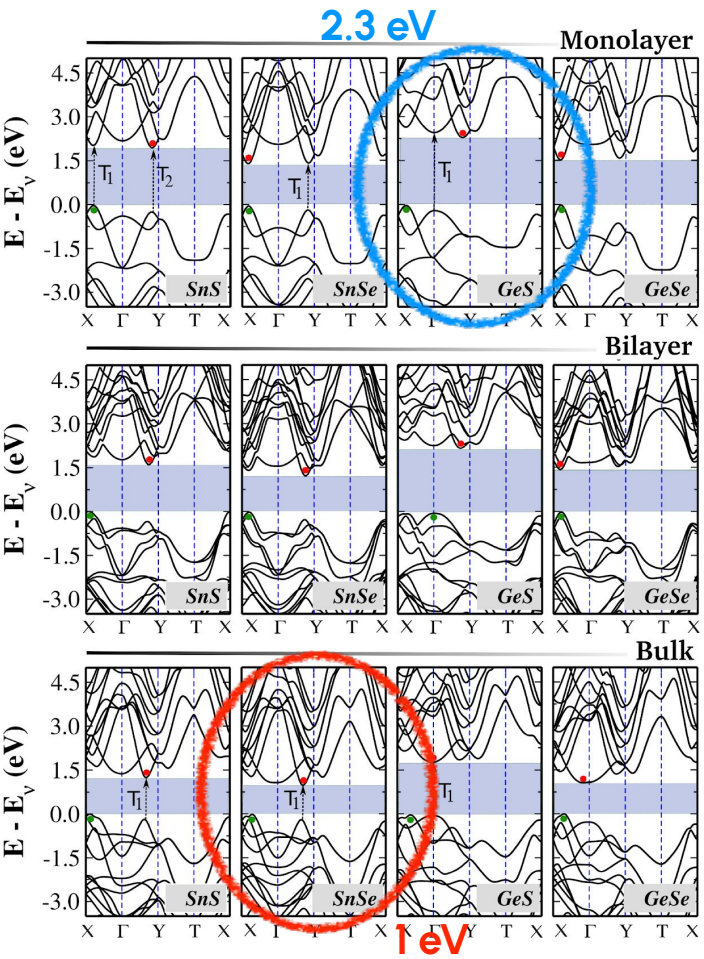






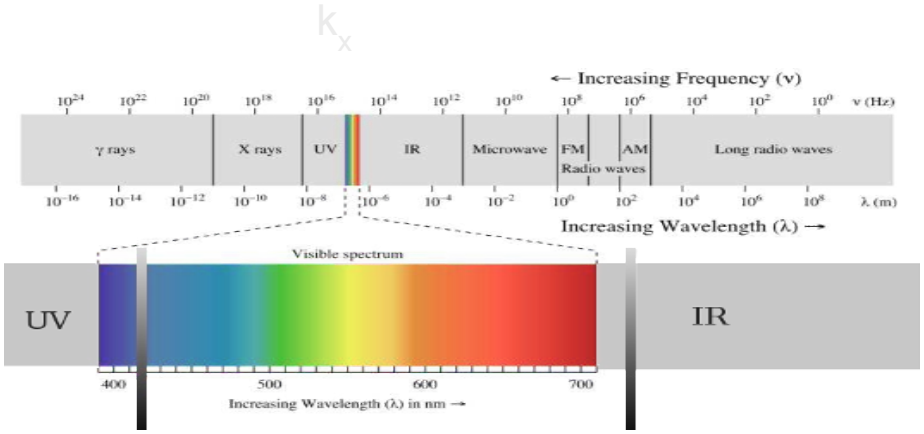
A..Splendiani, et. al, Nano Lett., 10, 2010

Band Gap Tuning: Group-IV Monochalcogenides



MX

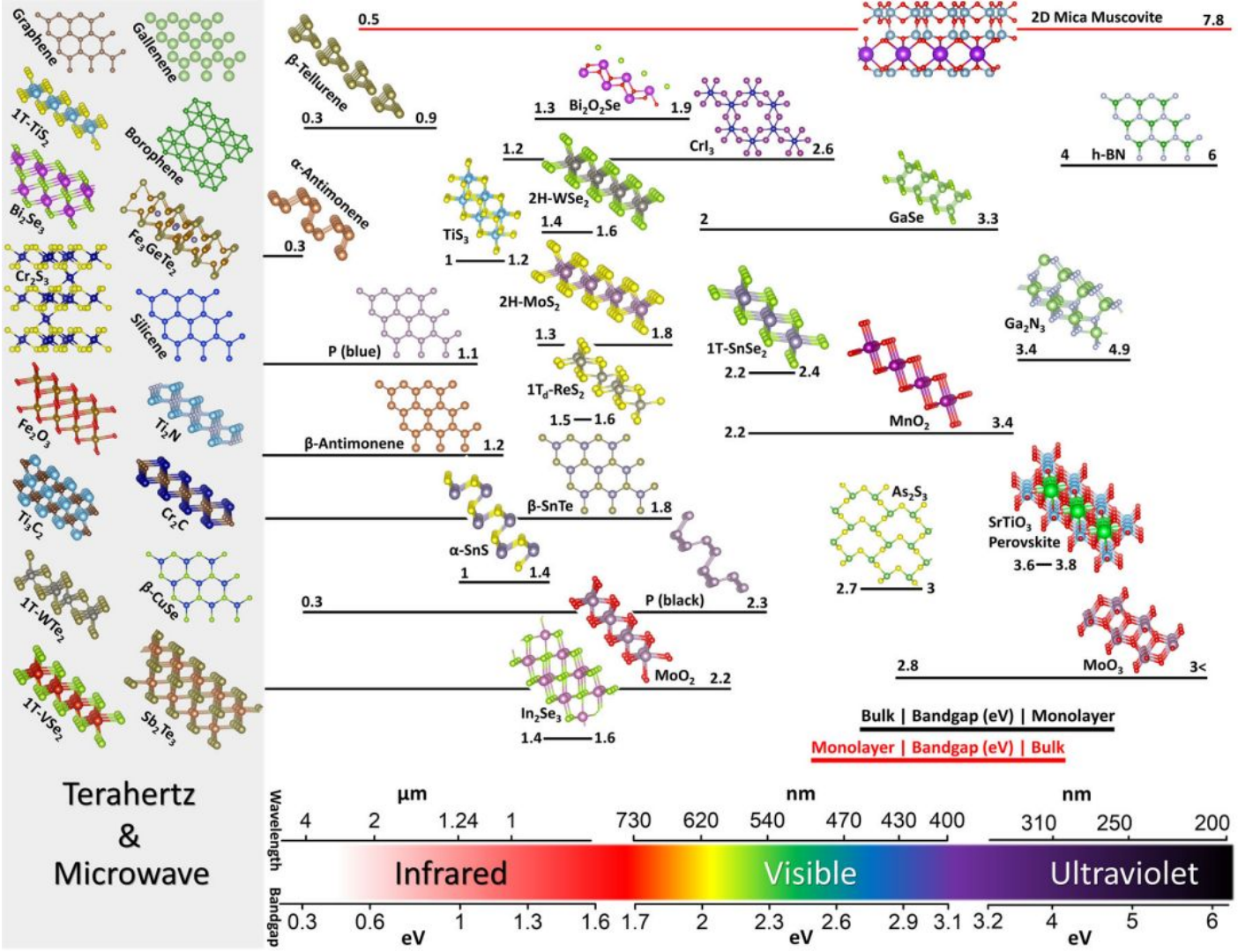
M = Sn, Ge, X = S, Se



2D GeS 3D SnSe

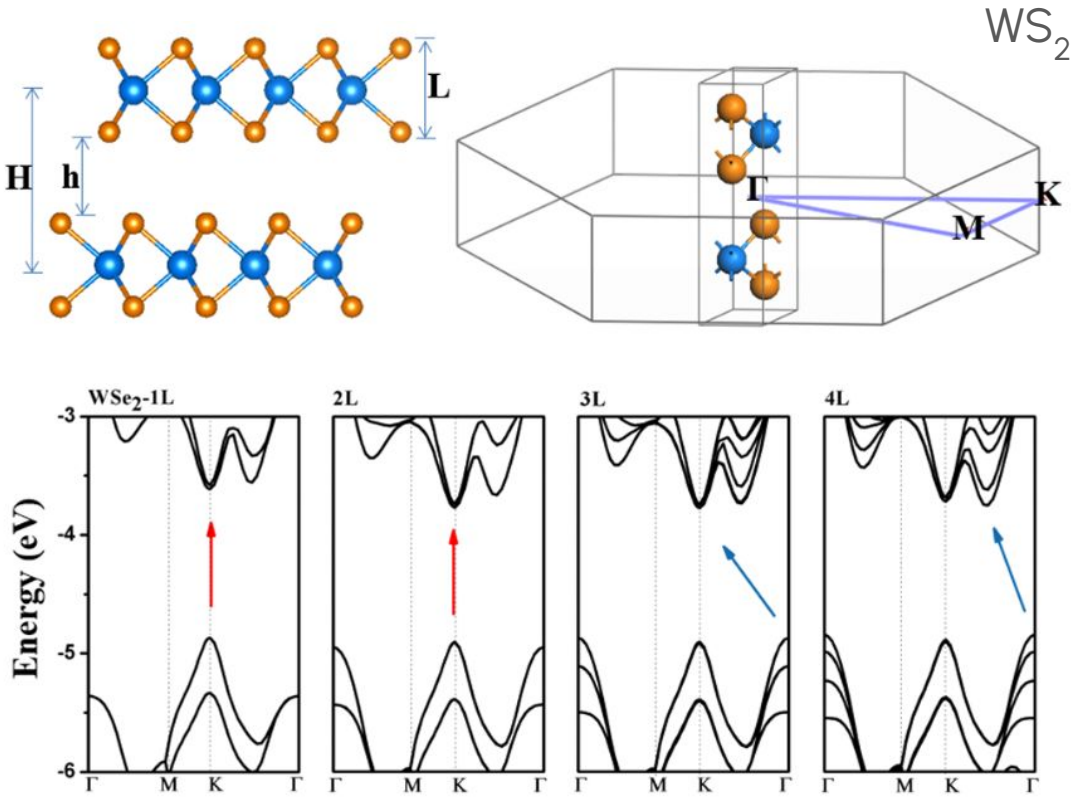
Gaps de energia cobrindo toda a região do visível.

Lídia Gomes and A. Carvalho, PRB, 92, 2015



A. Chaves, et al. npj 2D Mat. and Appl., 2020.

Band Gap Tuning: TMDCs



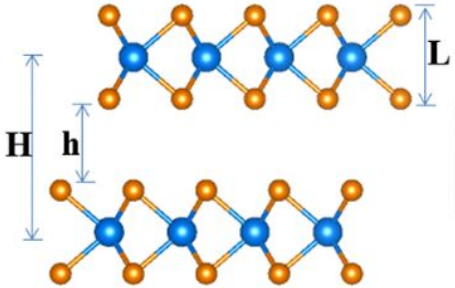
Y. Sun. et. al, J. Phys. Chem. C., 120, 2016

Spin Orbit Coupling (SOC)

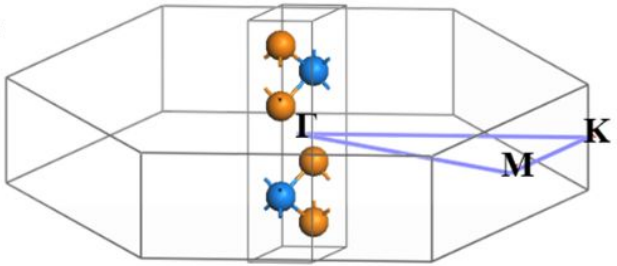
Relativistic interaction of a particle's spin with its motion inside a potential.

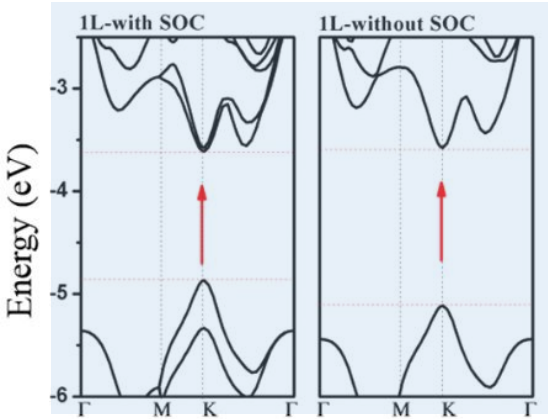
$$H_{SO} = \frac{1}{2m_e^2c^2}\frac{1}{r}\frac{dV(r)}{dr}\vec{S}\cdot\vec{L}$$

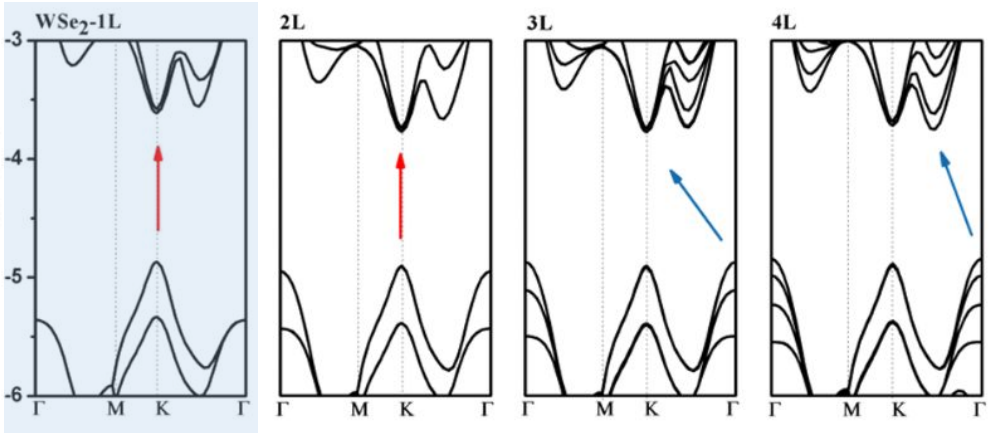
Band Gap Tuning: TMDCs

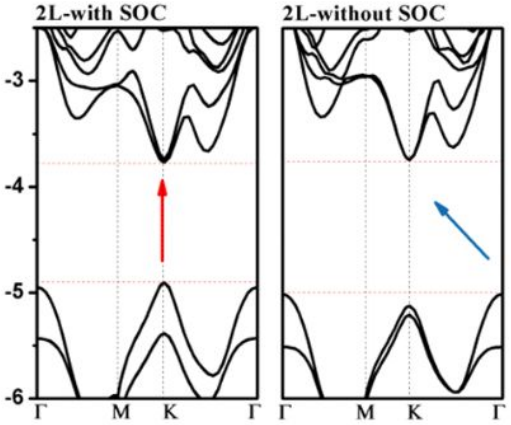


WS_2



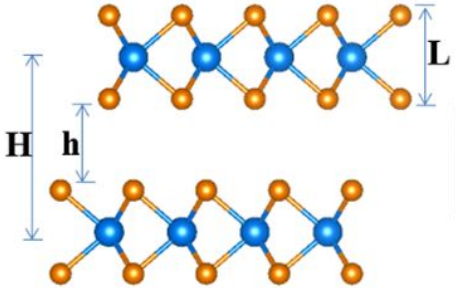


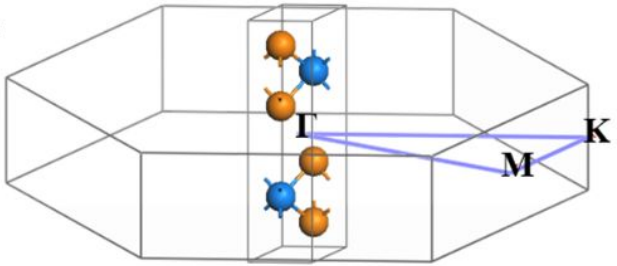


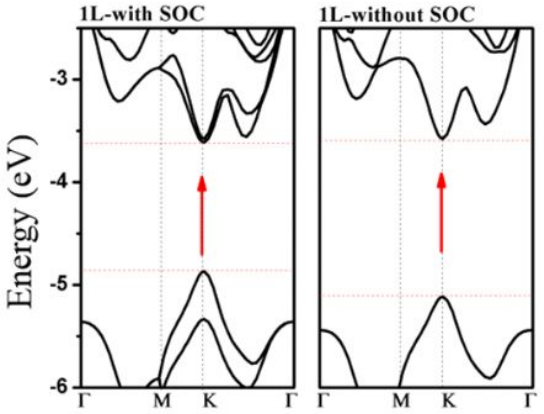


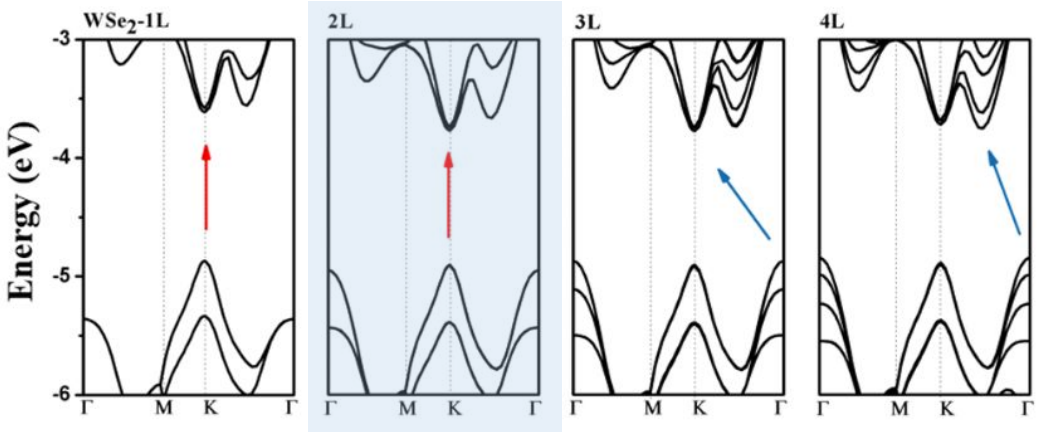
Y. Sun. et. al, J. Phys. Chem. C., 120, 2016

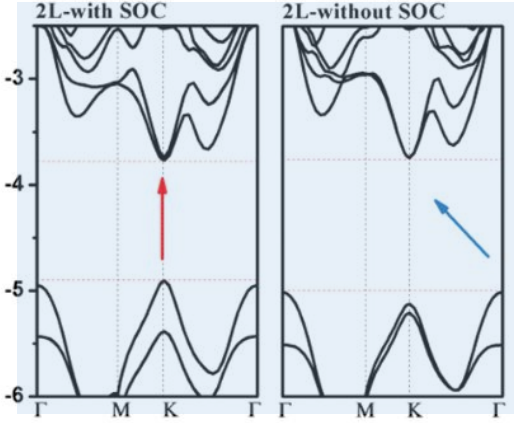
Band Gap Tuning: TMDCs











Y. Sun. et. al, J. Phys. Chem. C., 120, 2016

Spintronics

spin transport electronics

REVIEW

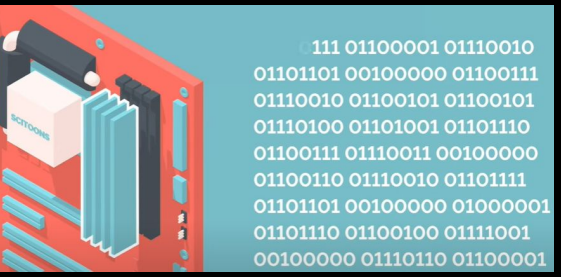
Spintronics: A Spin-Based Electronics Vision for the Future

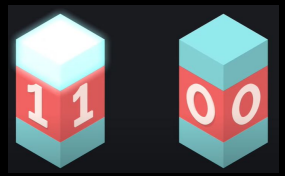
S. A. Wolf,[1,2*] D. D. Awschalom,[3] R. A. Buhrman,[4] J. M. Daughton,[5] S. von Molnár,[6] M. L. Roukes,[7] A. Y. Chtchelkanova,[8] D. M. Treger[8]

This review describes a new paradigm of electronics based on the spin degree of freedom of the electron. Either adding the spin degree of freedom to conventional charge-based electronic devices or using the spin alone has the potential advantages of nonvolatility, increased data processing speed, decreased electric power consumption, and increased integration densities compared with conventional semiconductor devices.

Major challenges in this field of spintronics that are addressed by experiment and

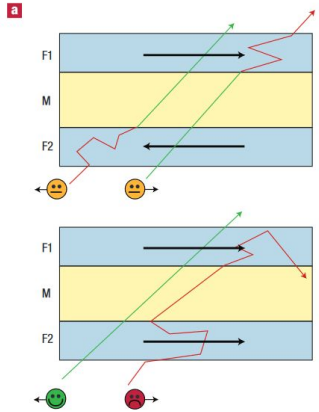
Electronics

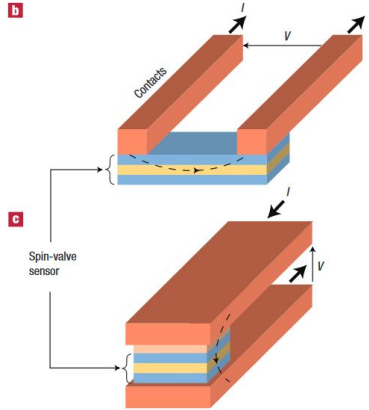




The emergence of spin electronics in data storage

Electrons have a charge and a spin, but until recently these were considered separately. In classical electronics, charges are moved by electric fields to transmit information and are stored in a capacitor to save it. In magnetic recording, magnetic fields have been used to read or write the information stored on the magnetization, which 'measures' the local orientation of spins in ferromagnets. The picture started to change in 1988, when the discovery of giant





npj | 2D Materials and Applications

REVIEW ARTICLE OPEN

2D materials for spintronic devices

Ethan C. Ahn[1]✉

2D materials are attractive for nanoelectronics due to their ultimate thickness dimension and variety of emerging spintronic device concepts will greatly benefit from the use of 2D materi manipulating spin. In this review, we discuss various 2D materials, including graphene and oth

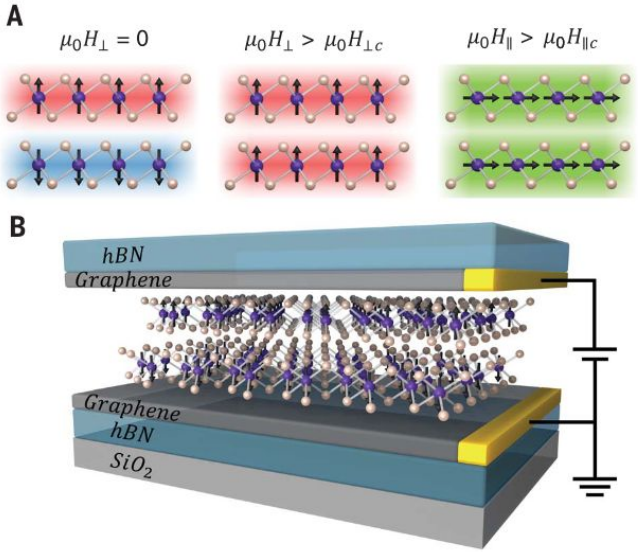
RESEARCH

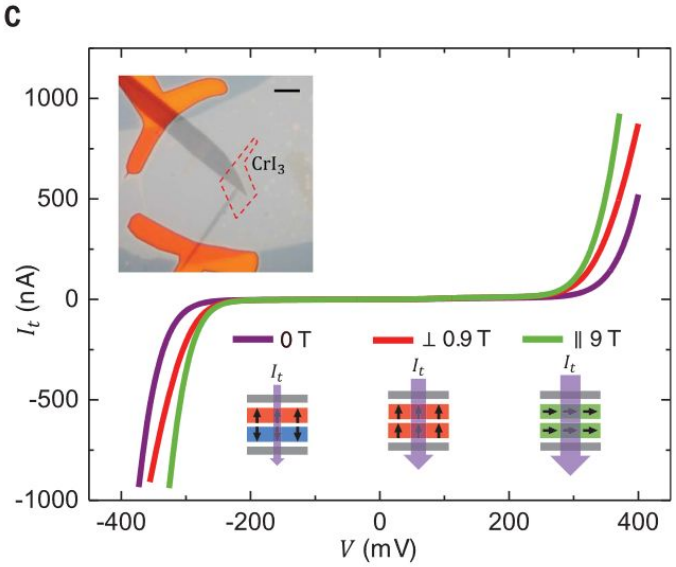
MAGNETISM

Giant tunneling magnetoresistance in spin-filter van der Waals heterostructures

Tiancheng Song[1]*, Xinghan Cai[1]*, Matisse Wei-Yuan Tu[2], Xiaoou Zhang[3], Bevin Huang[1], Nathan P. Wilson[1], Kyle L. Seyler[1], Lin Zhu[4], Takashi Taniguchi[5], Kenji Watanabe[5], Michael A. McGuire[6], David H. Cobden[1], Di Xiao[3]†, Wang Yao[2]†, Xiaodong Xu[1,4]†

Magnetic multilayer devices that exploit magnetoresistance are the backbone of magnetic sensing and data storage technologies. Here, we report multiple-spin-filter

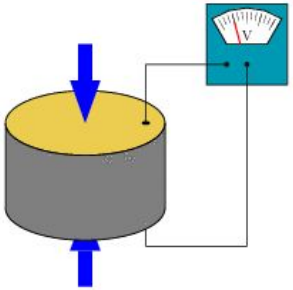


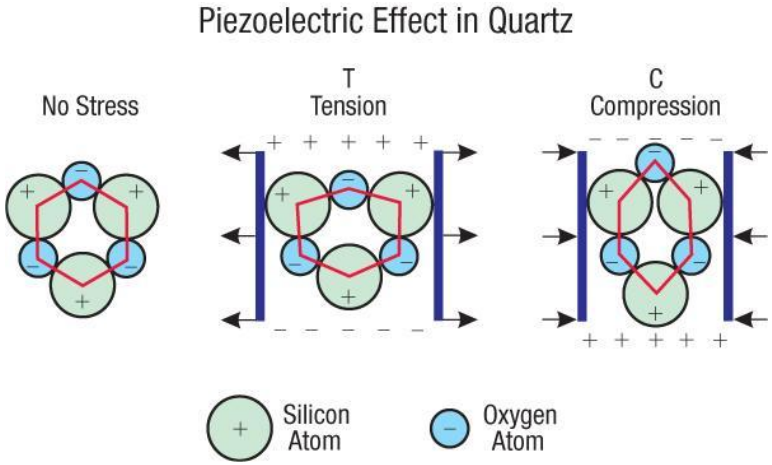


Song et al., Science 360, 1214, 2018.

Symmetry loss in 2D systems

Piezoelectricity



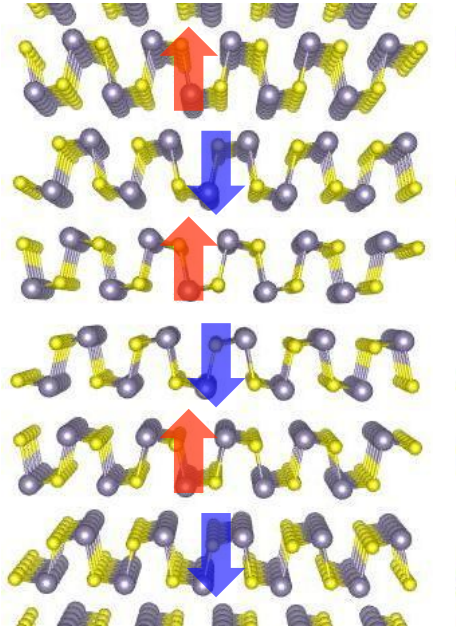


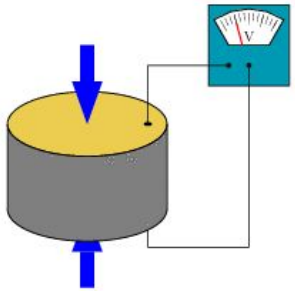
α-Quartz

SiO_4

Symmetry loss in 2D systems

Piezoelectricity





PHYSICAL REVIEW B **92**, 214103 (2015)

Enhanced piezoelectricity and modified dielectric screening of two-dimensional group-IV monochalcogenides

Lídia C. Gomes, A. Carvalho, and A. H. Castro Neto
Centre for Advanced 2D Materials and Graphene Research Centre, National University of Singapore, 6 Science Drive 2, 117546, Singapore
(Received 14 September 2015; revised manuscript received 16 November 2015; published 8 December 2015)

We use first-principles calculations to investigate the lattice properties of group-IV monochalcogenides.

$$e_{ij} = -\frac{\partial \sigma_i}{\partial E_j} = \frac{\partial P_i}{\partial \varepsilon_j}$$

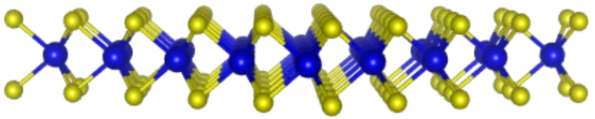
		Clamped-ion			Relaxed-ion		
		e_{32}^{2D}	e_{33}^{2D}	e_{24}^{2D}	e_{32}^{2D}	e_{33}^{2D}	e_{24}^{2D}
SnS	GGA-PBE	−4.73	0.29	−4.39	0.76	23.36	15.70
	vdW-TS	−5.01	0.47	−4.75	2.27	18.94	15.54
SnSe	GGA-PBE	−4.89	0.53	−4.67	4.42	24.18	28.17
	vdW-TS	−4.67	0.58	−4.29	6.73	30.25	30.82
GeS	GGA-PBE	−6.69	−1.25	−7.10	−4.97	7.28	0.37
	vdW-TS	−6.89	−0.81	−7.08	−4.64	8.83	2.05
GeSe	GGA-PBE	−7.16	−0.26	−7.37	−3.00	13.26	8.25
	vdW-TS	−7.11	0.35	−7.20	−1.48	16.95	12.48
h-BN		−3.71	3.71		−1.38	1.38	
MoS_2		−3.06	3.06		−3.64	3.64	
$MoTe_2$		−2.98	2.98		−5.43	5.43	

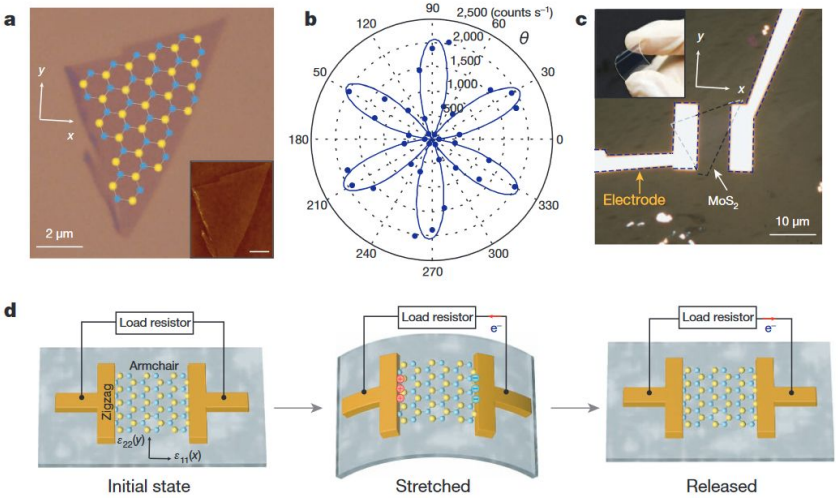
Symmetry loss in 2D systems

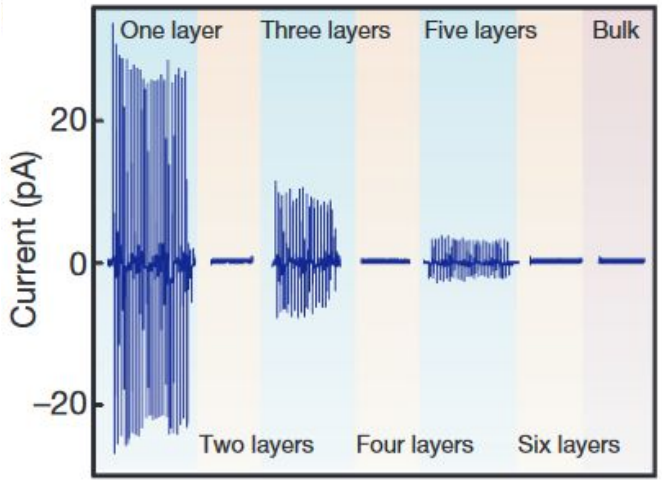
Piezoelectricity

Piezoelectricity of single-atomic-layer MoS_2 for energy conversion and piezotronics

Wenzhuo Wu[1]*, Lei Wang[2]*, Yilei Li[3], Fan Zhang[4], Long Lin[1], Simiao Niu[1], Daniel Chenet[4], Xian Zhang[4], Yufeng Hao[4], Tony F. Heinz[3], James Hone[4] & Zhong Lin Wang[1,5]





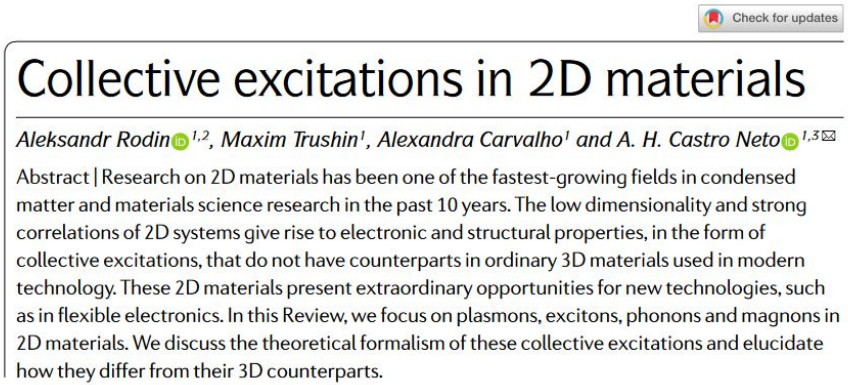


Muitas (todas?) propriedades interessantes dos materiais 2D surgem devido às fortes **correlações eletrônicas**.

↓

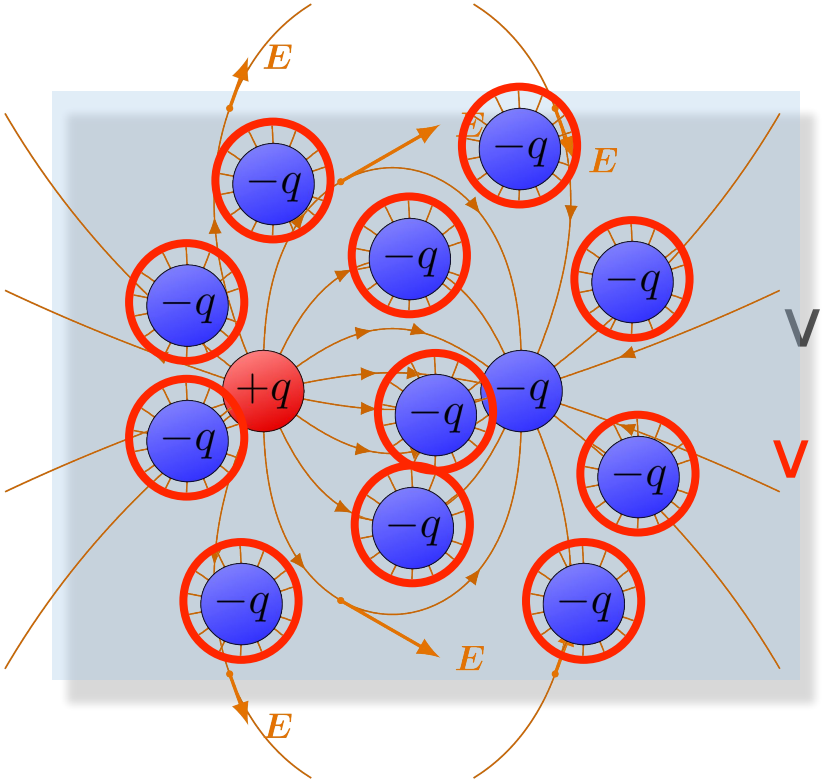
Modos coletivos!

REVIEWS



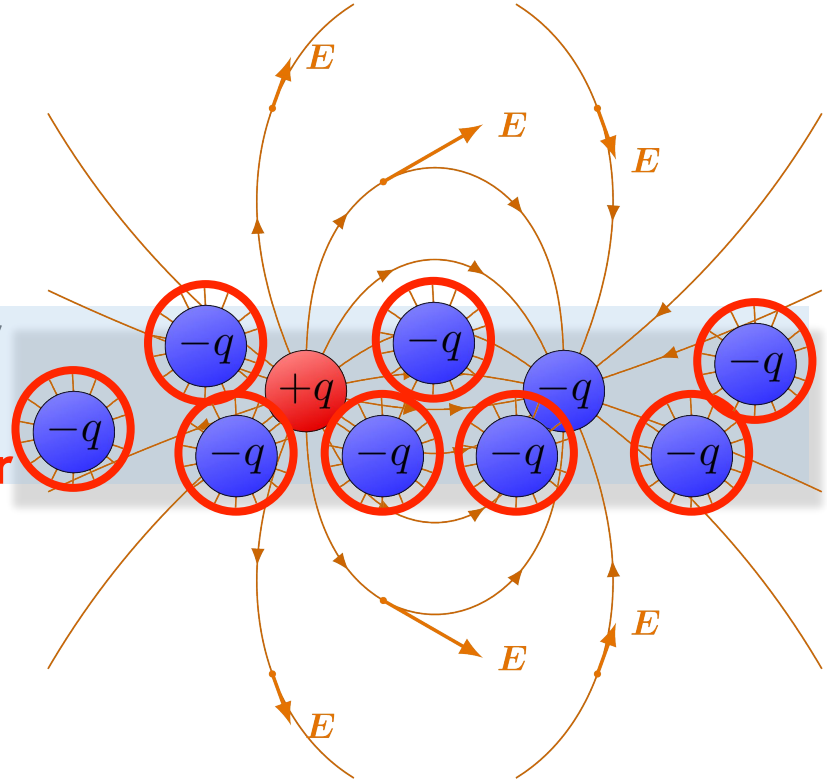
New properties due to high electronic correlation

Poor screening in 2D systems



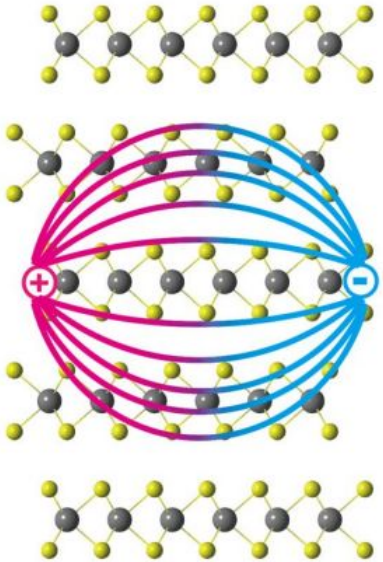
$V \propto q^2/r$

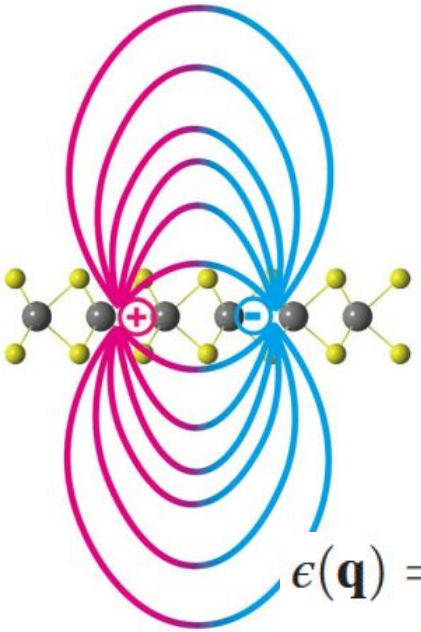
$V \propto q^2/\varepsilon r$



https://tikz.net/electric_fieldlines2/

Modified Coulomb potential in 2D systems



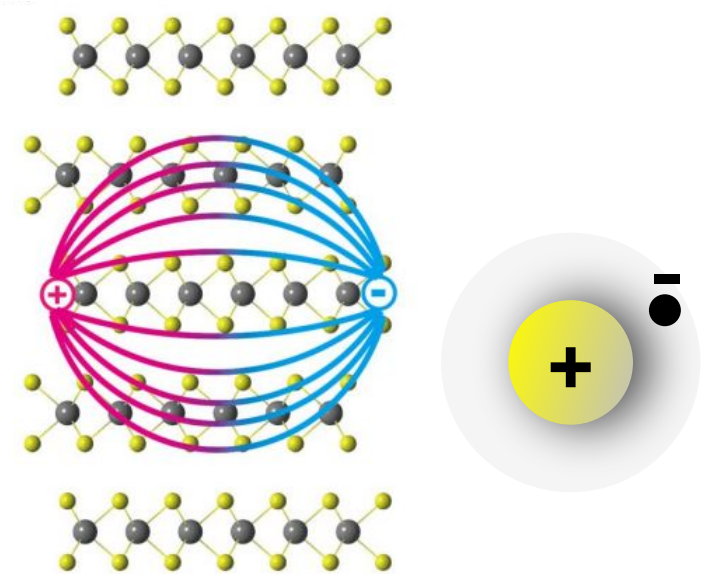


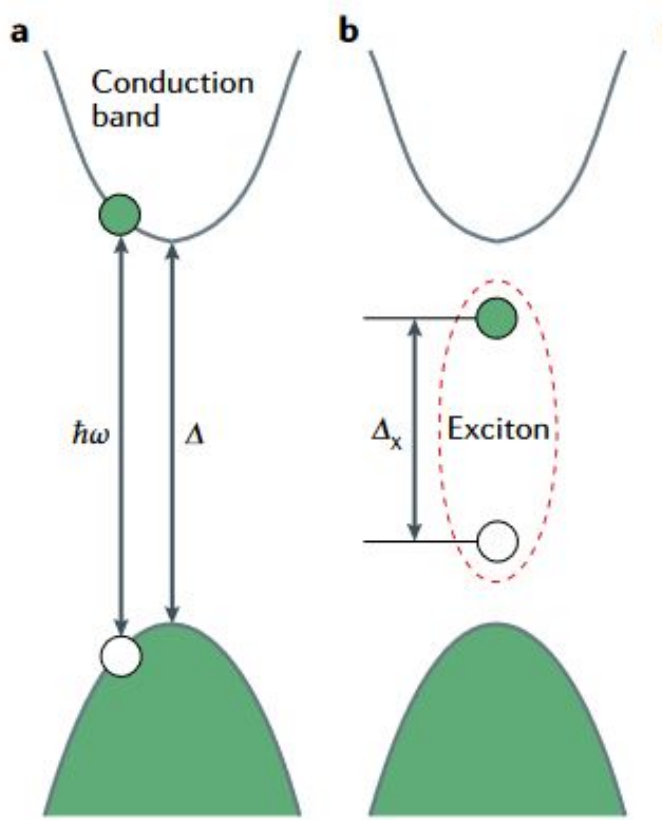
$$\epsilon(\mathbf{q}) = 1 + 2\pi\alpha q$$

$$V_{3D} = \frac{e}{4\pi\varepsilon_r\varepsilon_0 r}$$

$$V_{2D}(r, z = 0) = -\frac{e^2}{8\varepsilon_0 r_0}\left[H_0\left(\frac{\varepsilon_r r}{r_0}\right) - Y_0\left(\frac{\varepsilon_r r}{r_0}\right)\right]$$

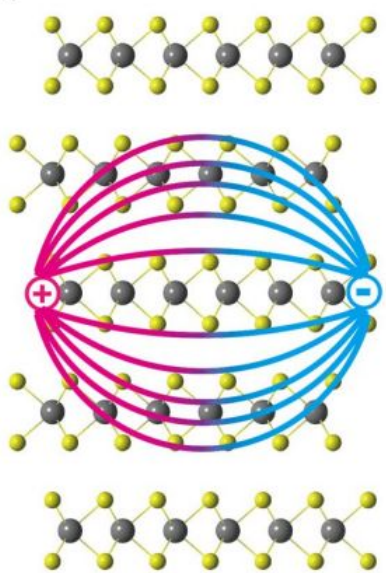
Excitons

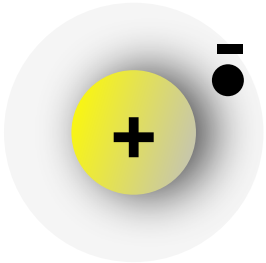




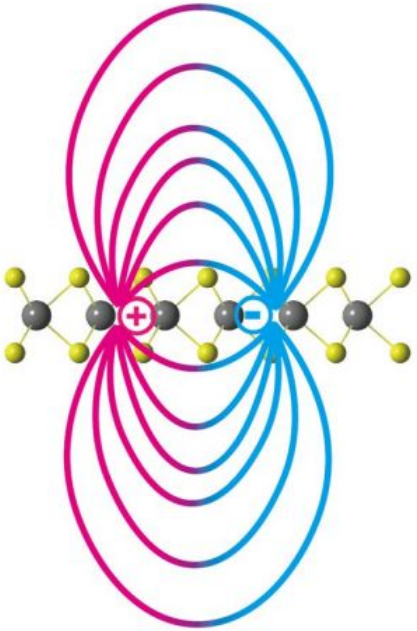
J. Hwang et al.,Sci. Report, 10, 2020

Excitons





$$\epsilon(\mathbf{q}) = 1 + 2\pi\alpha q$$



J. Hwang et al.,Sci. Report, 10, 2020

Exciton Binding Energy and Nonhydrogenic Rydberg Series in Monolayer WS_2

Alexey Chernikov,[1,*] Timothy C. Berkelbach,[2] Heather M. Hill,[1] Albert Rigosi,[1] Yilei Li,[1] Burak Aslan,[1] David R. Reichman,[2] Mark S. Hybertsen,[3] and Tony F. Heinz[1,†]

[1]*Departments of Physics and Electrical Engineering, Columbia University, 538 West 120th Street, New York, New York 10027, USA*
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[3]*Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, New York 11973-5000, USA*

(Received 12 March 2014; published 13 August 2014)

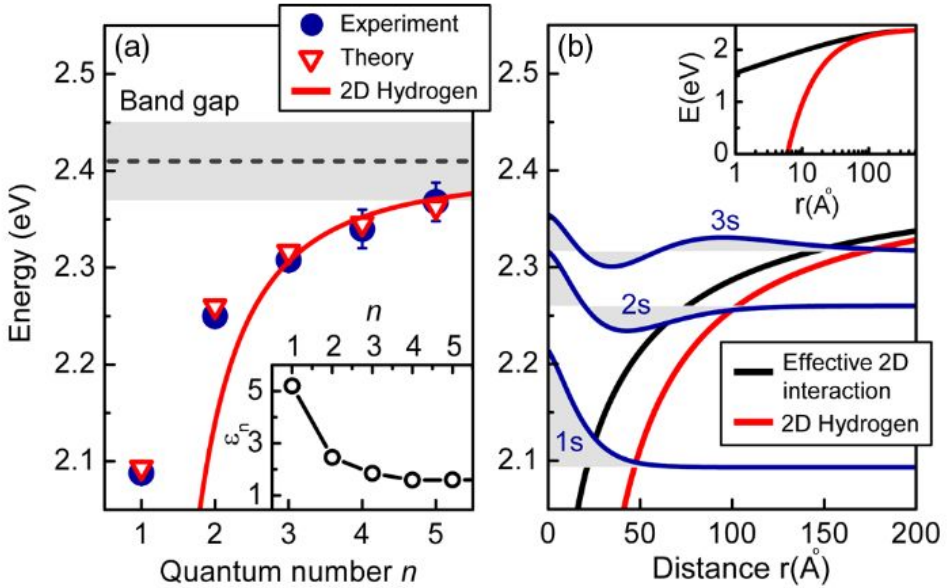
We have experimentally determined the energies of the ground and first four excited excitonic states of the fundamental optical transition in monolayer WS_2, a model system for the growing class of atomically thin two-dimensional semiconductor crystals. From the spectra, we establish a large exciton binding energy

$$V_{eh}(r) = -e^2/\varepsilon r$$

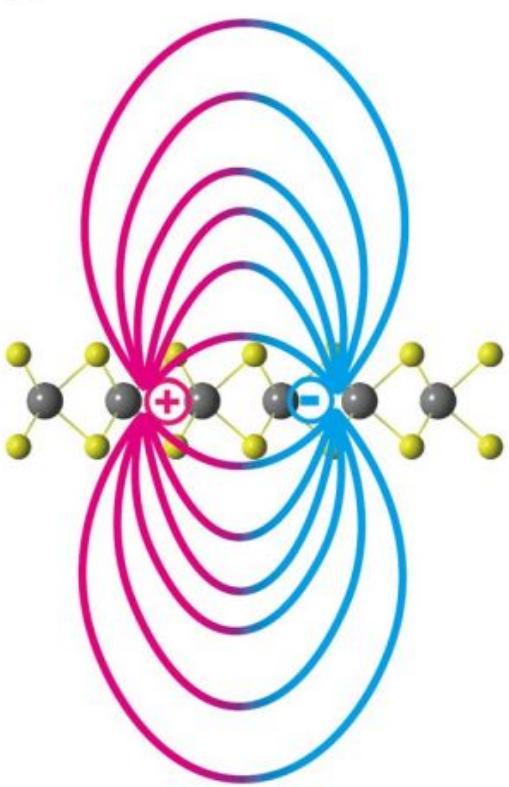
$$E_b^{(n)} = \frac{\mu e^4}{2\hbar^2\varepsilon^2(n-1/2)^2}$$

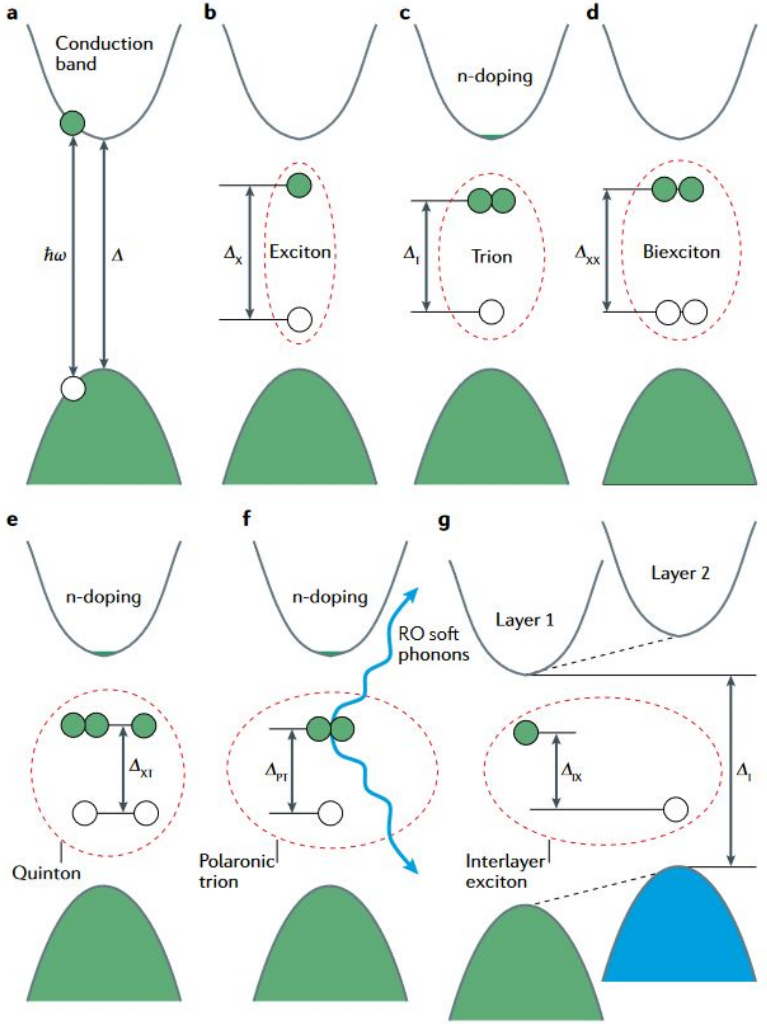
$$\epsilon(\mathbf{q}) = 1 + 2\pi\alpha q$$

$$V_{eh}(r) = -\frac{\pi e^2}{2r_0}\left[H_0\left(\frac{r}{r_0}\right) - Y_0\left(\frac{r}{r_0}\right)\right]$$



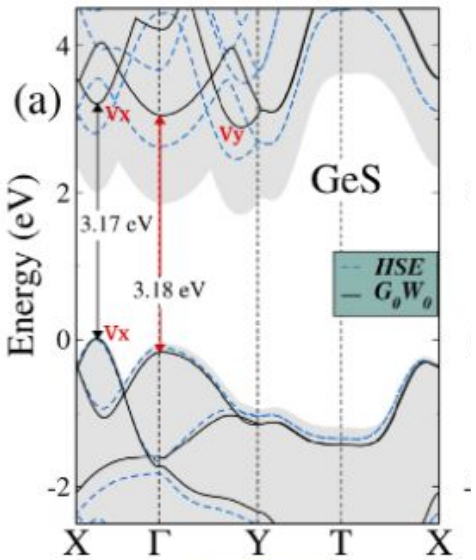
Excitons

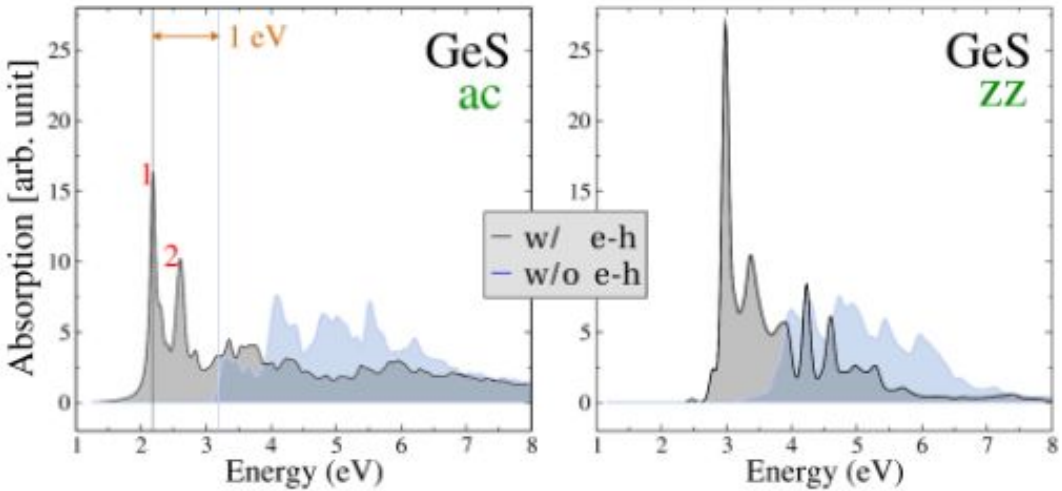


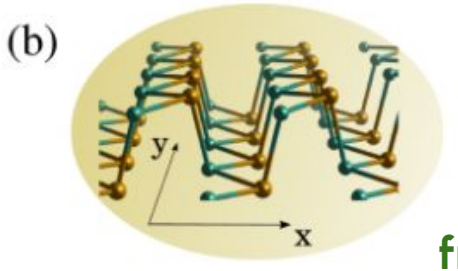


Alex. Rodin, Nature Rev., 2, 2020.

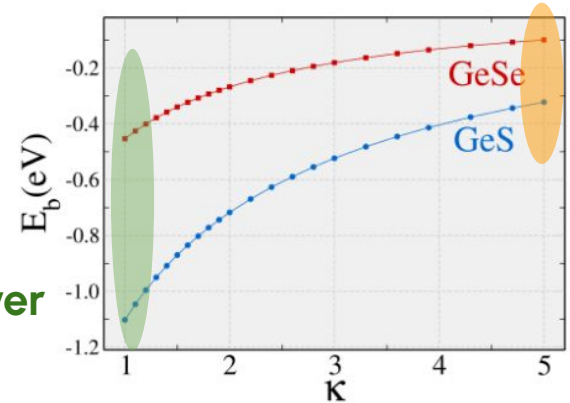
Excitons: Group IV-Monochalcogenides







free standing layer



on top of a substrate

Topological excitations: Skyrmions, Merons

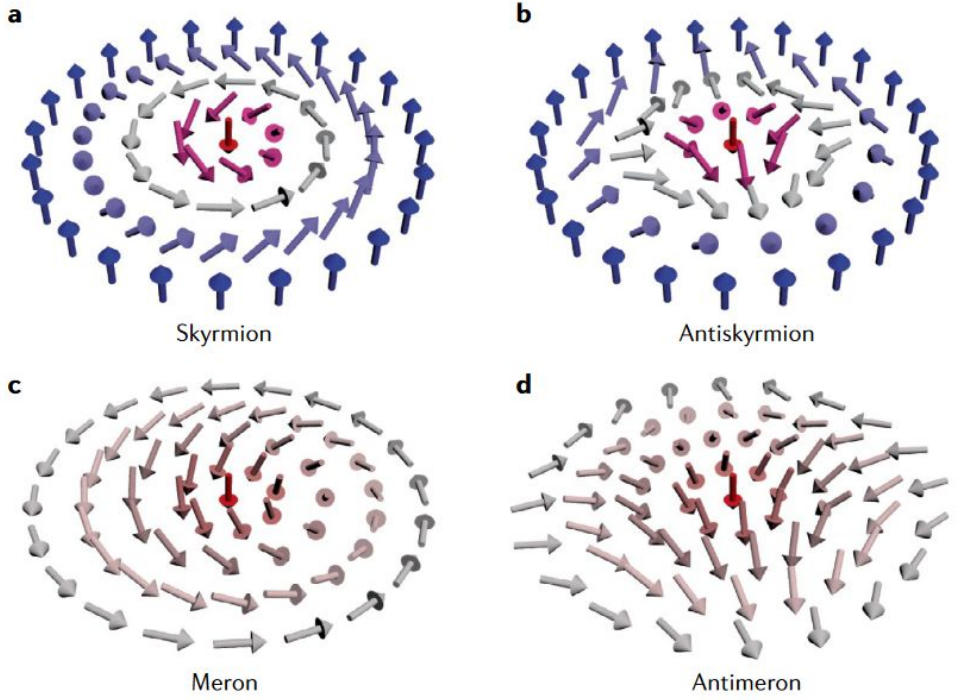


Fig. 7 | **Chiral magnetic spin textures. a** | Skyrmion (spiral-type), topological charge $Q=-1$. **b** | Antiskyrmions, topological charge $Q=+1$. **c** | Meron, topological charge $Q=-1/2$. **d** | Antimeron, topological charge $Q=+1/2$. Reprinted from REF.[148], Springer Nature Limited.

Alex. Rodin, Nature Rev., 2, 2020.