2D Materials

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Bilkent University

2D Materials: Graphene

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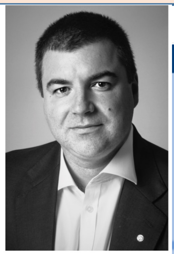
Andre Geim
Prize share: 1/2



© The Nobel Foundation. Photo: U. Montan
Konstantin Novoselov
Prize share: 1/2

PRESSMEDDELANDE
Press release

5 October 2010

The Nobel Prize in Physics 2010

The Royal Swedish Academy of Sciences has decided to award the Nobel Prize in Physics for 2010 to

Andre Geim and **Konstantin Novoselov**

University of Manchester, UK — University of Manchester, UK

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

Graphene – the perfect atomic lattice

A thin flake of ordinary carbon, just one atom thick, lies behind this year's Nobel Prize in Physics. Andre Geim and Konstantin Novoselov have shown that carbon in such a flat form has exceptional properties that originate from the remarkable world of quantum physics.

When mixed into plastics, graphene can turn them into conductors of electricity while making them more heat resistant and mechanically robust. This resilience can be utilised in new super strong materials, which are also thin, elastic and lightweight. In the future, satellites, airplanes, and cars could be manufactured out of the new composite materials.

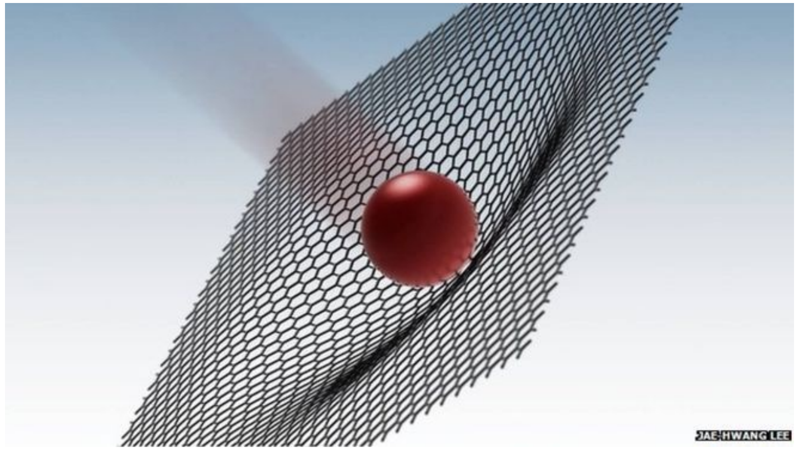
https://www.nobelprize.org/prizes/physics/2010/summary/

https://www.nobelprize.org/uploads/2018/06/press-9.pdf

Zheng, Qingbin et al. *Materials Today* 36 (2020): 158-179

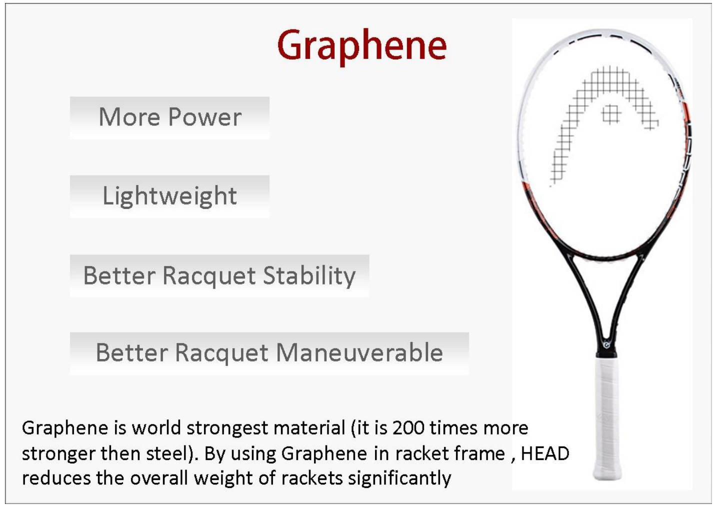
2D Materials: Graphene

- Properties
  - strongest material ever tested
  - very flexible
  - very light
  - efficiently conducts heat and electricity
  - nearly transparent
  - zero-gap semiconductor



Bulletproof graphene
J. Lee, P. E. Loya, J. Lou, E. L. Thomas, Science, 346, 2014, 1092

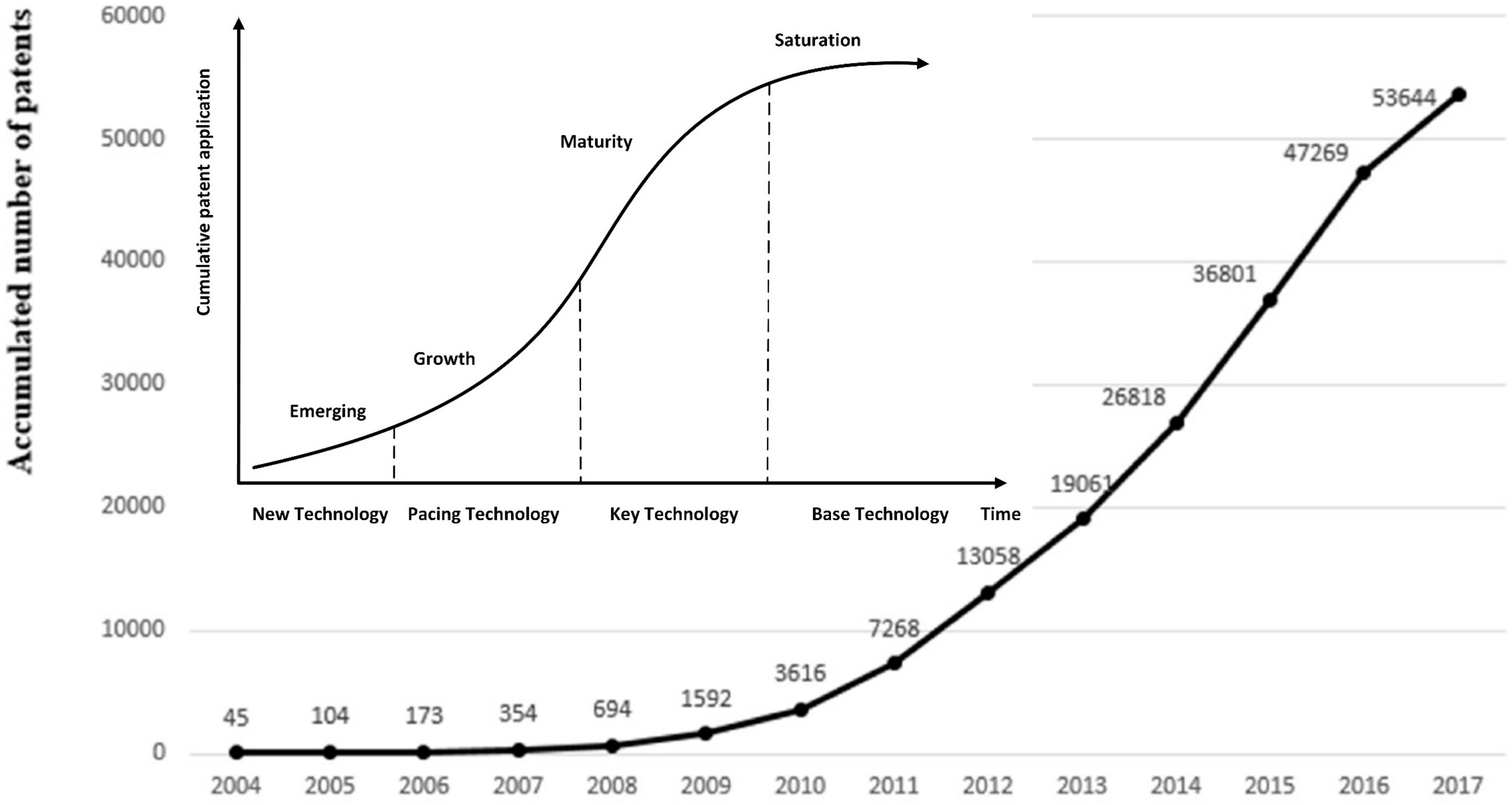
flexible displays
https://newatlas.com/graphene-led-display-flexible-electronics/35884/

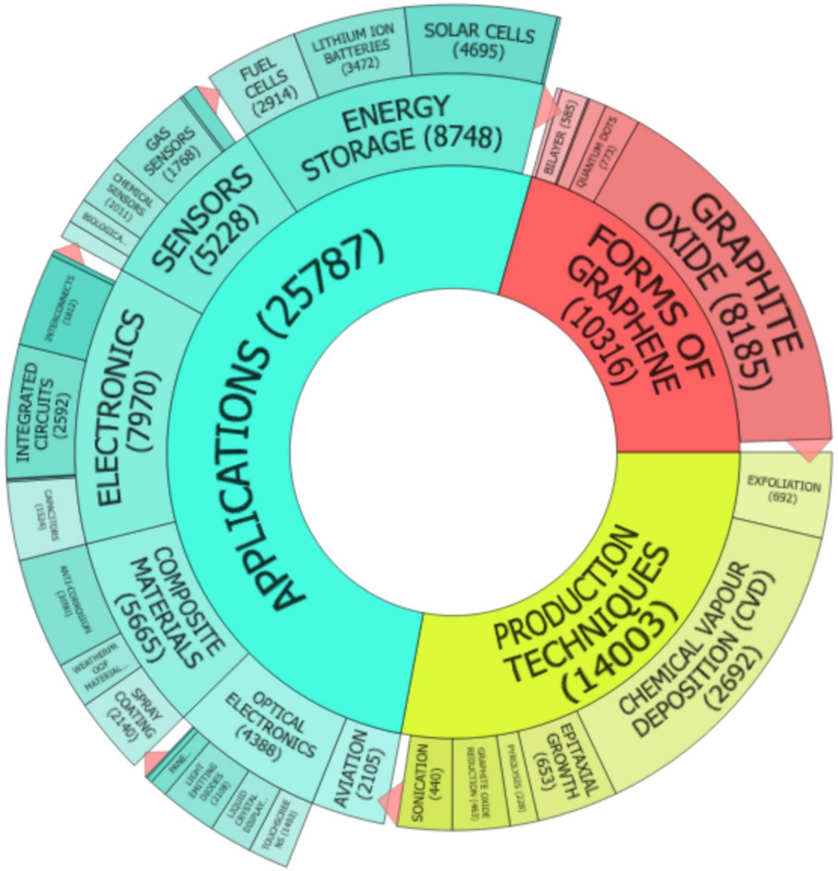


Catlike has managed to incorporate Graphene nano-fibers into the manufacturing of cycling helmets, giving the head of cyclists maximum protection with minimum weight.

2D Materials: Graphene

- Patents (Publication year range 2004 to 2017)
  - ➢Number of patent publications 49912
  - ➢Number of patent families 30963
  - ➢Top Applicant Samsung Electronics Co Ltd



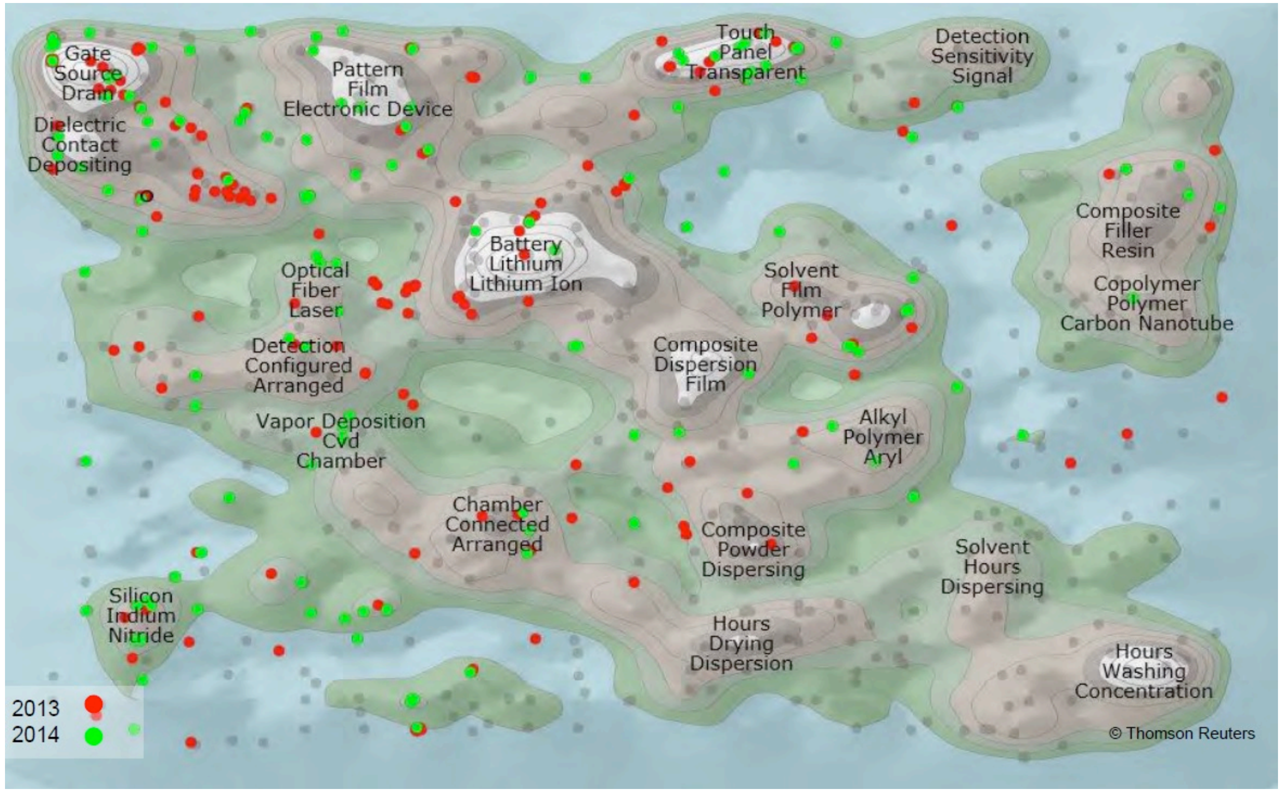


https://patentanalysis.org/graphene-patent-analysis-study/

Yang Xi *et al.*, Sustainability **2018**, 10, 4800

2D Materials: Graphene

- Samsung (top patent applicant)
  - Interested in graphene because it is highly flexible, incredible strong and is a good conductor of heat making it the perfect material for use in flexible displays and wearables, something Samsung is betting on heavily with devices like the Gear Fit fitness tracker it launched at Mobile World Congress.
  - The Samsung Advanced Institute of Technology (SAIT), in partnership with South Korea's Sungkyunkwan University (SKKU) have announced a new breakthrough in the mass manufacturing techniques for graphene, the substance that is widely expected to take over from silicon as the material of choice in next generation electronics.
  - It's hoped that this manufacturing process could drastically reduce the cost of creating large quantities of graphene which is still prohibitively expensive for use in consumer electronics.

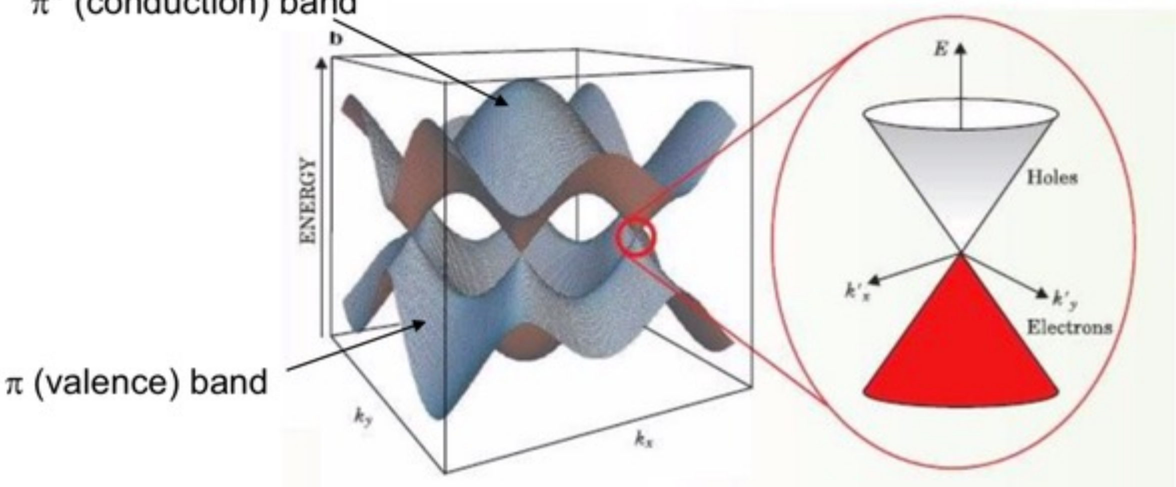


Graphene patent landscape map highlighting Samsung patents.
focus: energy storage, flexible electronics

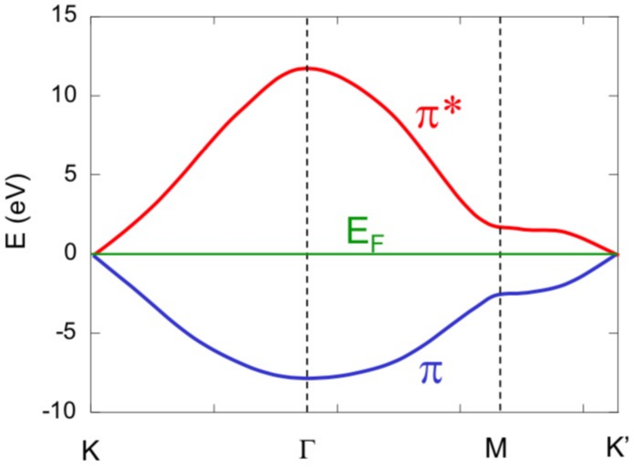
http://www.htxt.co.za/2014/04/07/samsung-makes-graphene-breakthrough/

3D band structure of graphene sheet

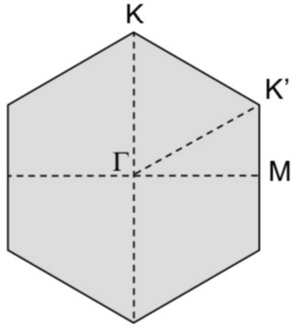
3D-band structure

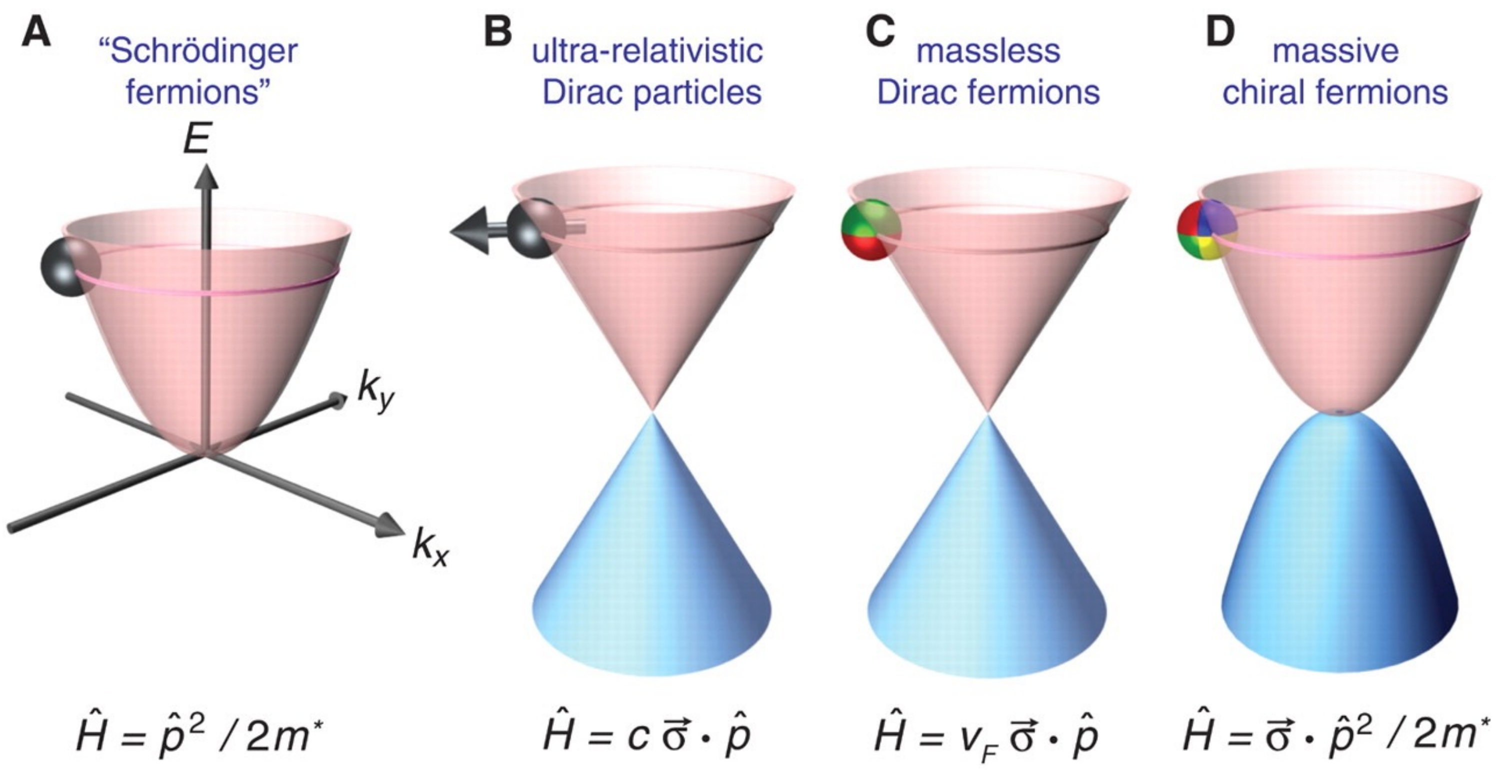


Projected energy band structure

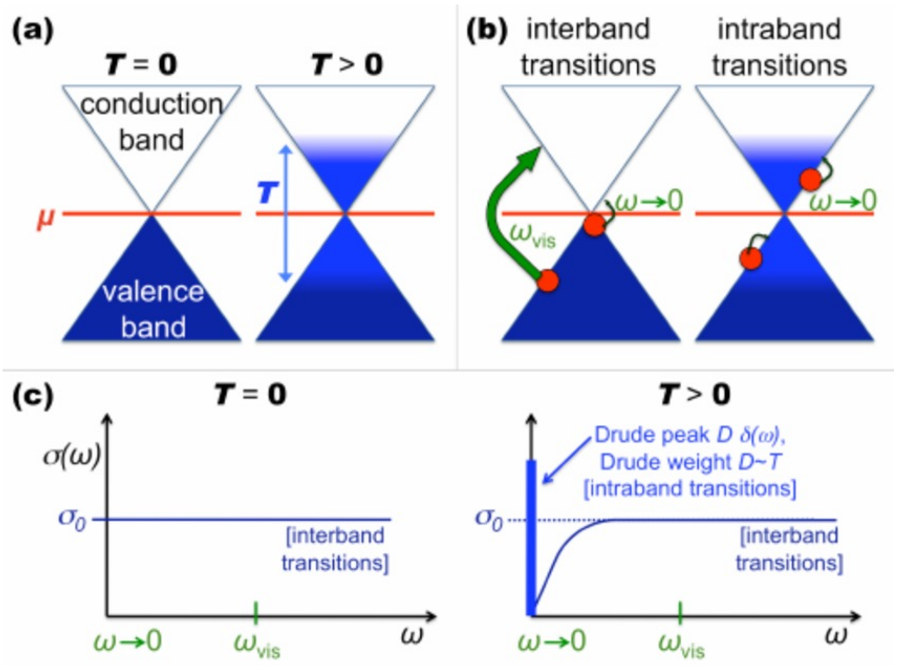


First-Brillouin zone of graphene





Science 19 Jun 2009: Vol. 324, Issue 5934, pp. 1530-1534 DOI: 10.1126/science.1158877

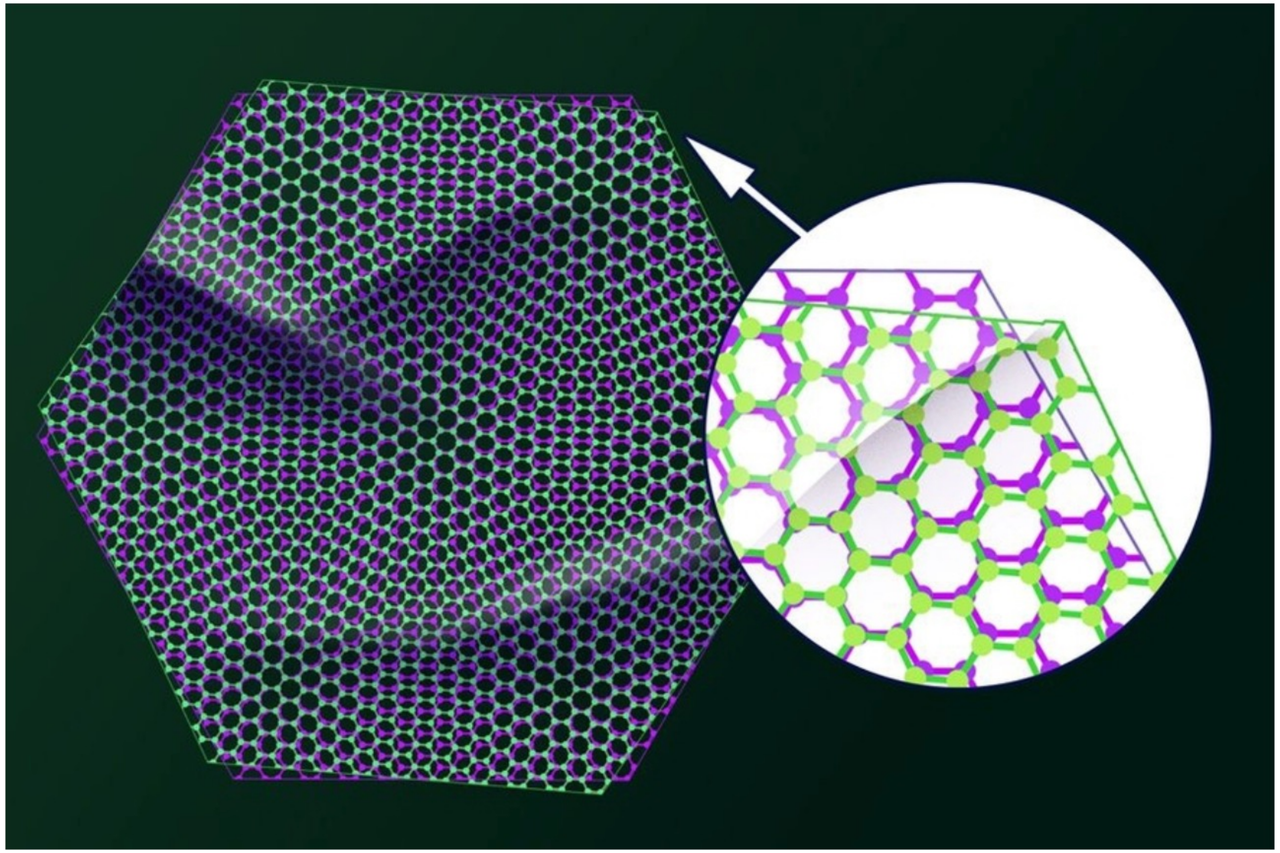


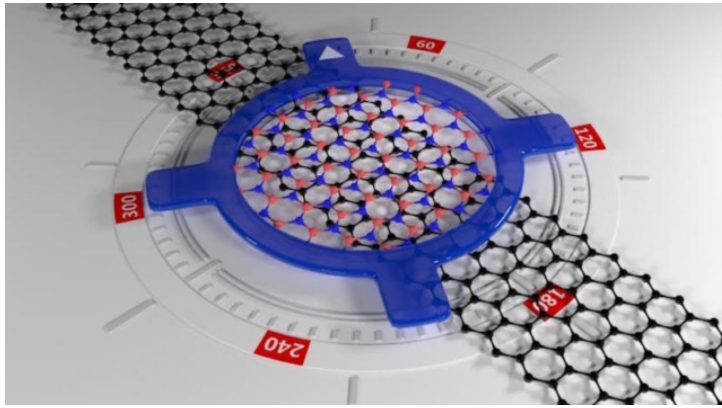
Charge carriers in graphene are called massless Dirac fermions and are described by a 2D analog of the Dirac equation, with the Fermi velocity *v*F ≈ 1 × 106 m/s playing the role of the speed of light

Graphene Magic Angle

Researchers map tiny twists in "magic-angle" graphene

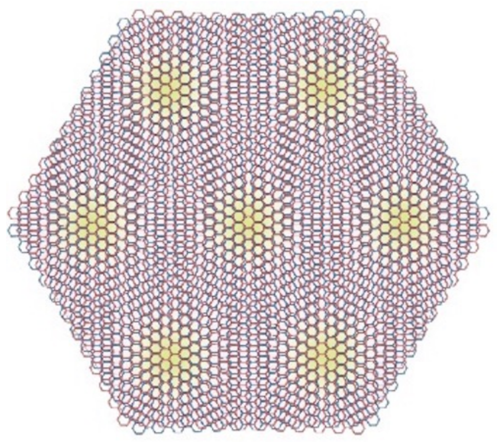
Results could help designers engineer high-temperature superconductors and quantum computing devices.





In this illustration, two sheets of graphene are stacked together at a slightly offset "magic" angle, which can become either an insulator or superconductor. "We placed one sheet of graphene on top of another, similar to placing plastic wrap on top of plastic wrap," MIT professor Pablo Jarillo-Herrero says. "You would expect there would be wrinkles, and regions where the two sheets would be a bit twisted, some less twisted, just as we see in graphene."

Image: José-Luis Olivares, MIT

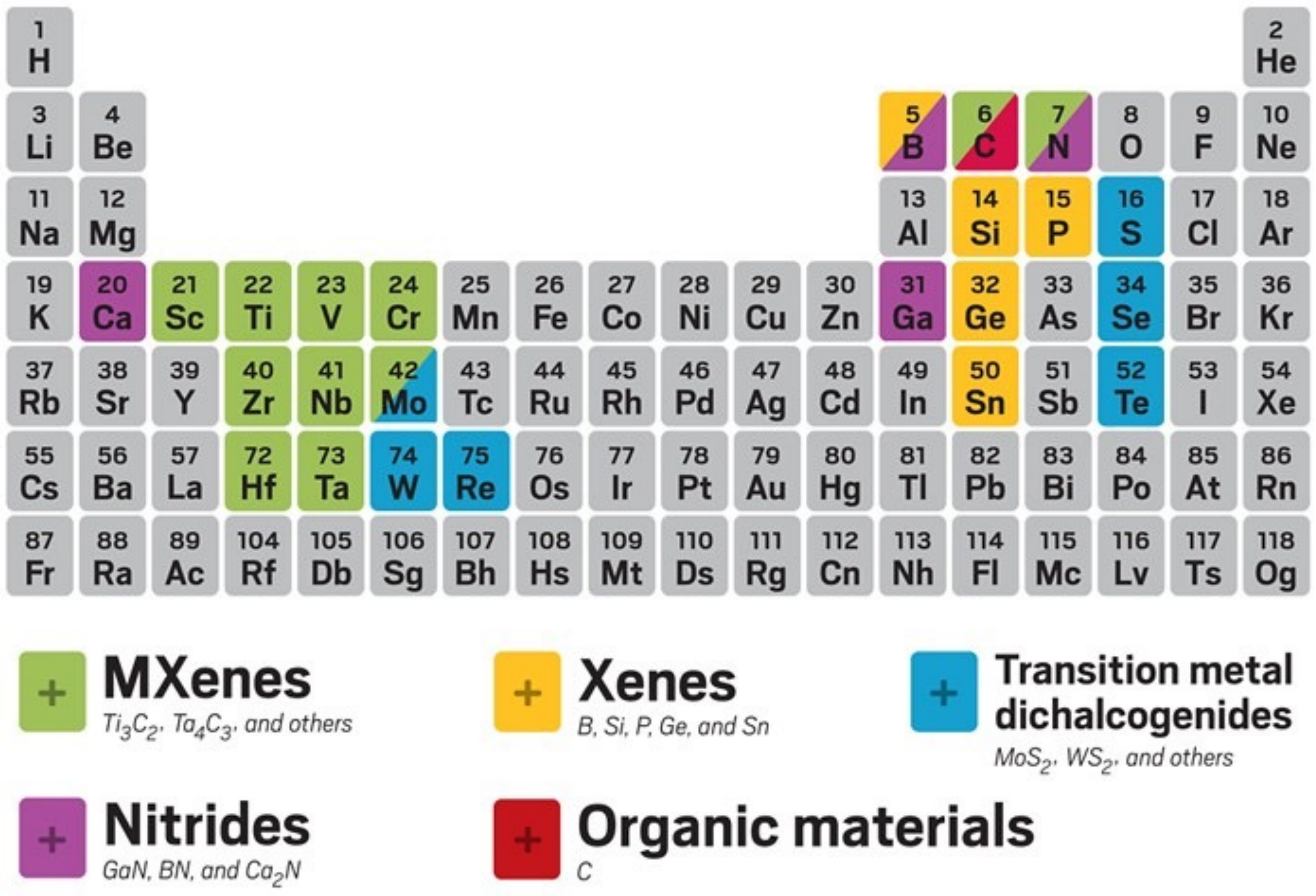


Twistronics' tunes 2D material properties

https://news.mit.edu/2020/twists-magic-angle-graphene-map-0508

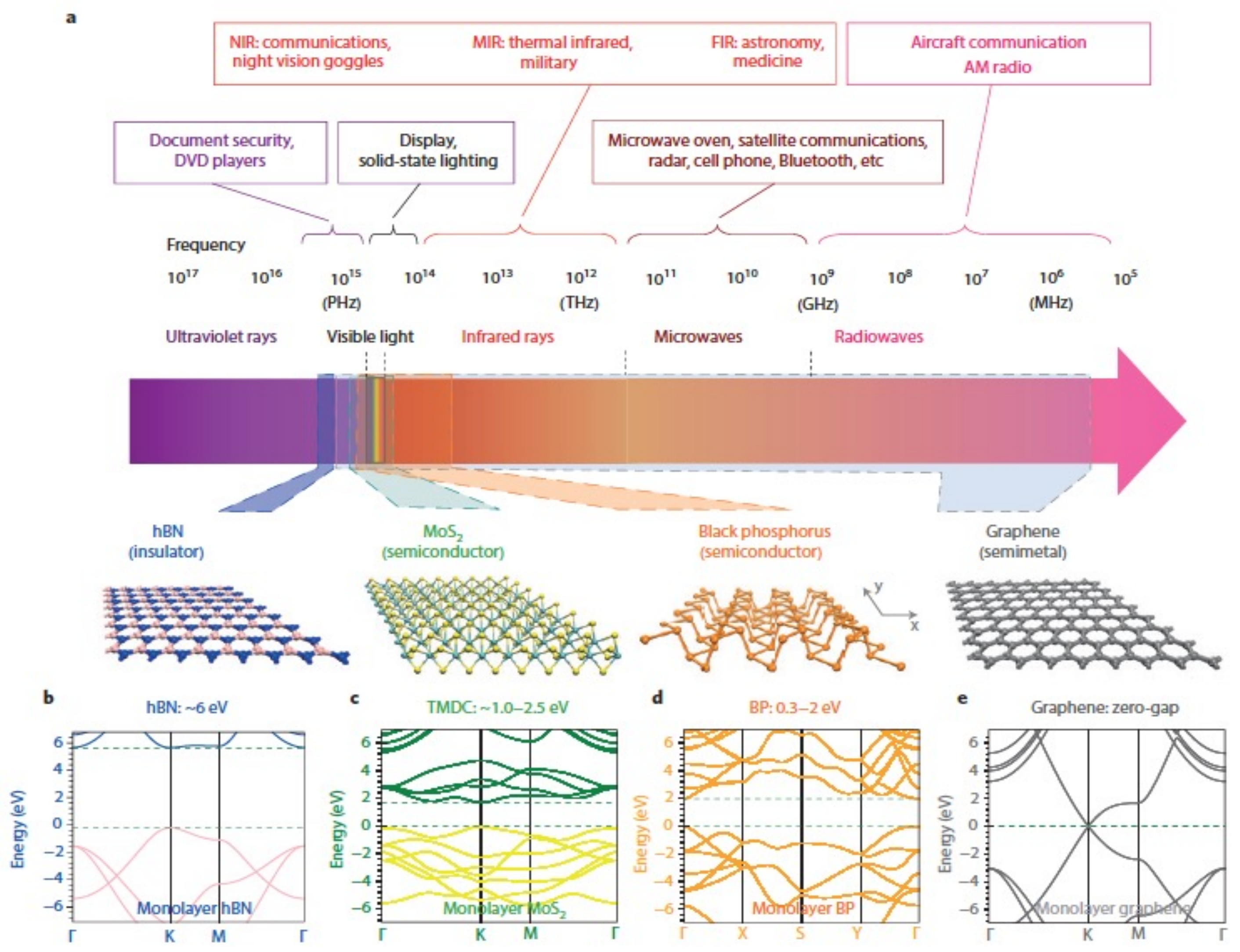
2D Materials: Beyond Graphene

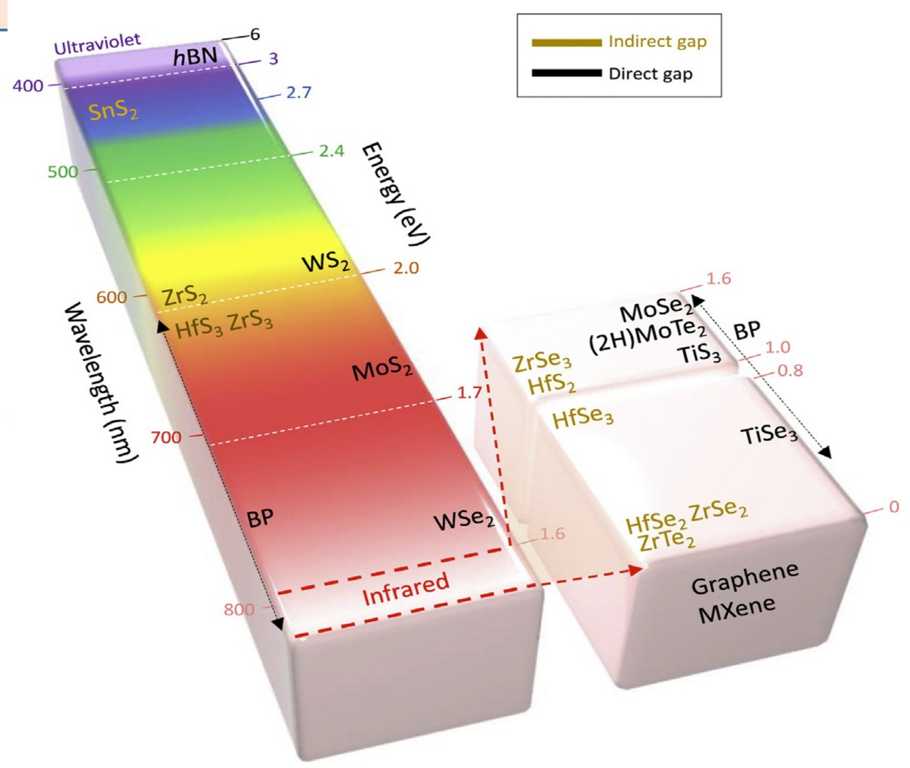
- Cons:
    - no bandwidth
    - very hydrophobic
    - very expensive and hard to manufacture
    - hard to produce in large usable sheets.
- Other 2D materials
    - MXenes
    - TMDCs
    - Silicene
    - h-BN etc.
- Heterostructures
    - Graphene/MXene
    - Graphene/TMDC
    - Graphene/h-BN
    - etc.



https://cen.acs.org/articles/95/i22/2-D-materials-beyond-graphene.html

2D Materials: Beyond Graphene

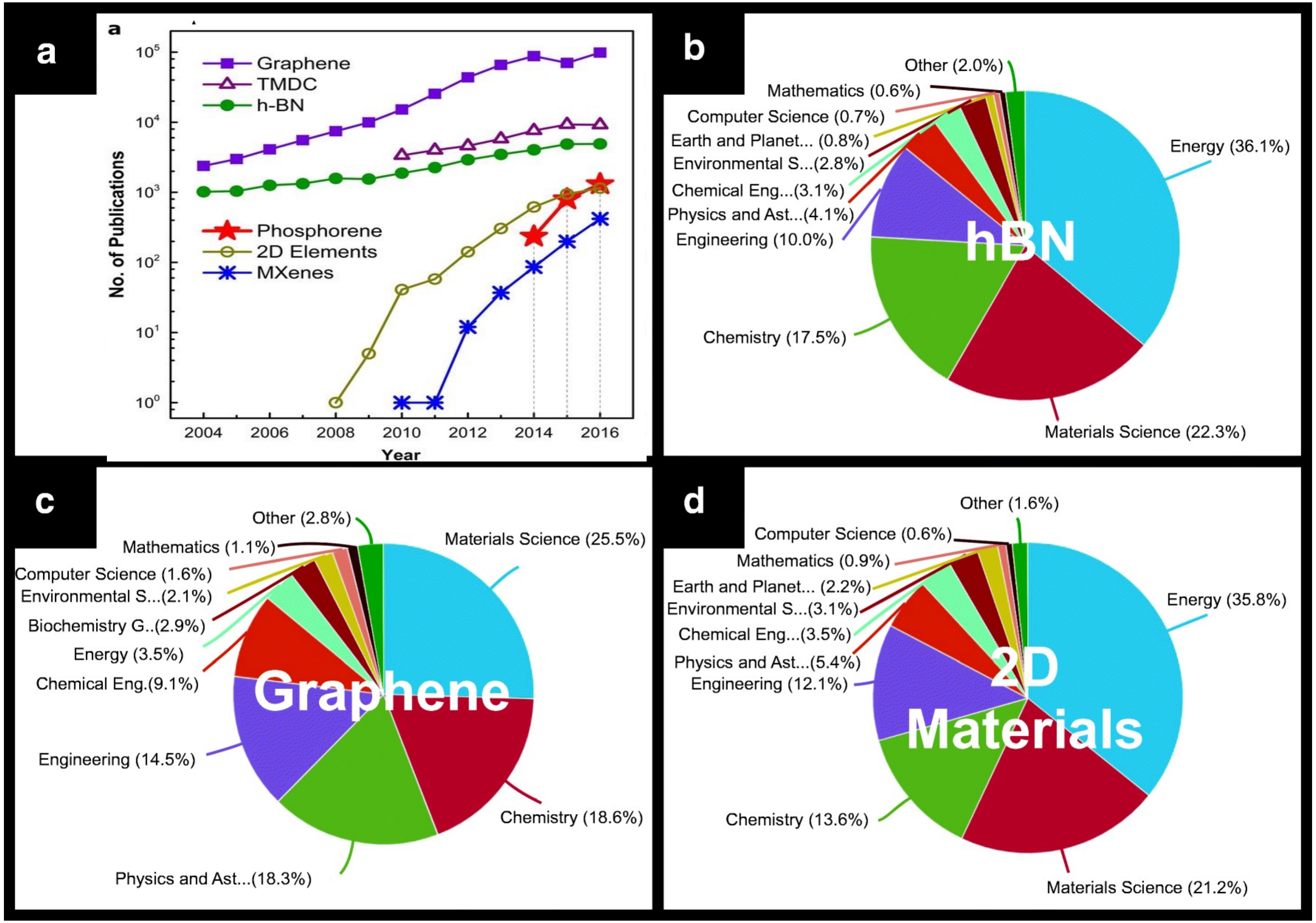




F. Xia, et al. Nat. Photonics 8 (2014) 899–907
S. Lin, et al. Sci. Rep. 5 (2015) 1510
W. Wu, et al. Nature 514 (2014) 470
N. Choudhary, et al. J. Mater. Chem. A 3 (2015) 24049
H. Li, et al. Small 8 (2012) 63
S. Cui, et al. Nat. Commun. 6 (2015) 8632
D. Sarkar, et al. ACS Nano 8 (2014) 3992
W. Choi et al. Materials Today 20 (2017), 3

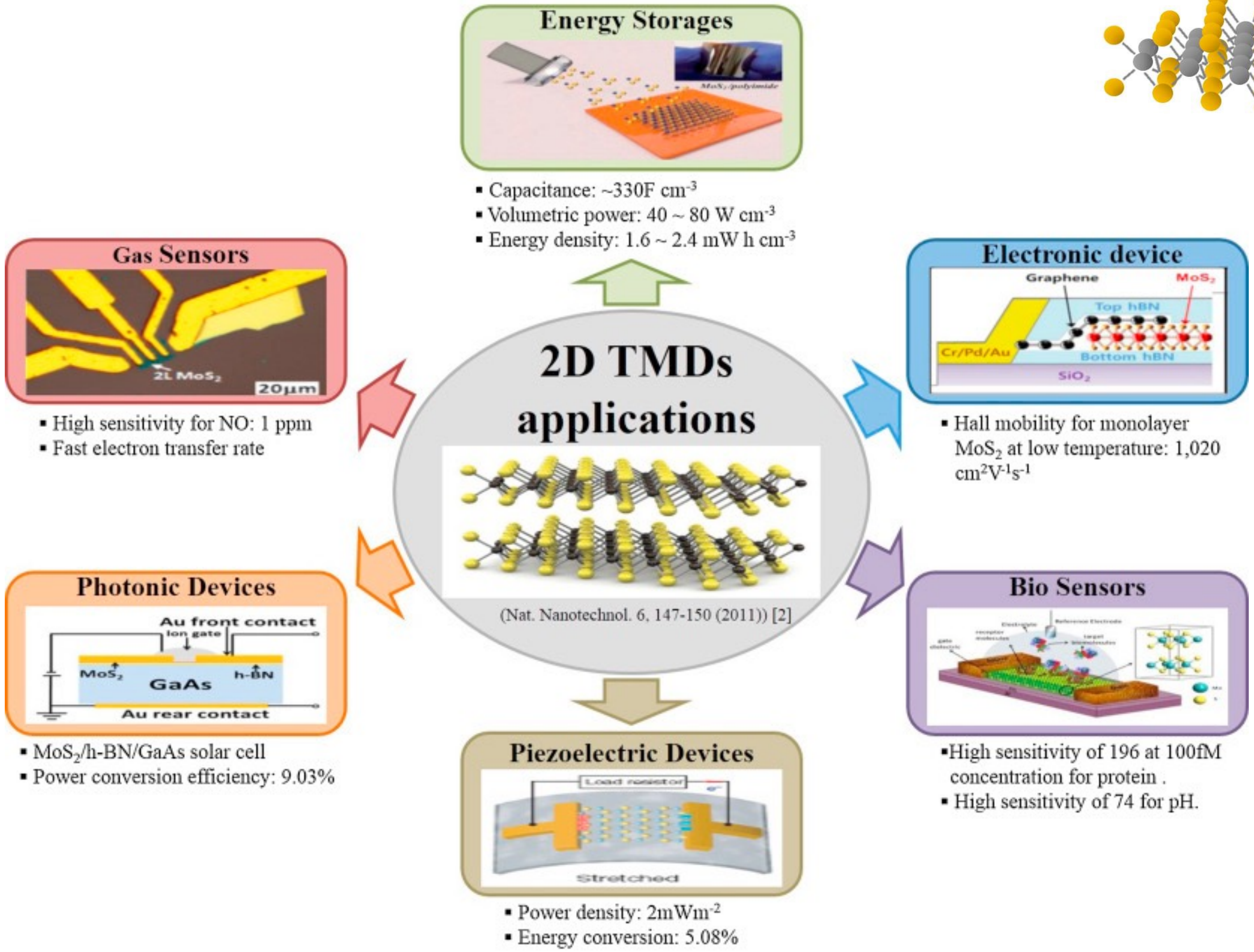
Graphene and 2D Materials

M. Akhtar et al., Npj 2D Mater. Appl. **1**, 5 (2017)



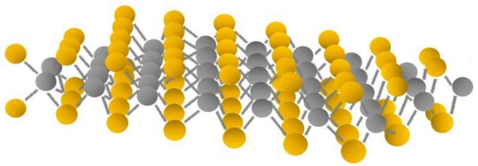
Garcia-Miranda Ferrari, A., et al. (2021). Analytical and Bioanalytical Chemistry, 413(3), 663-672.

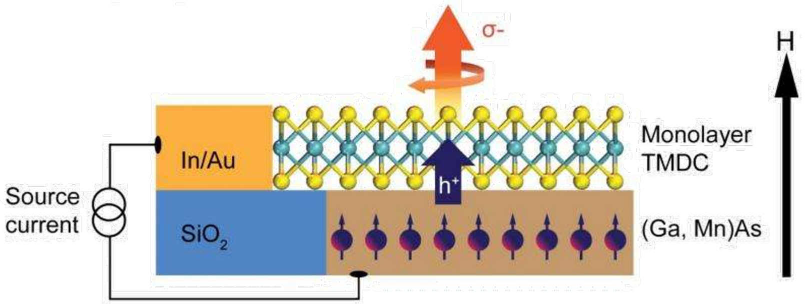
2D Materials: TMDCs



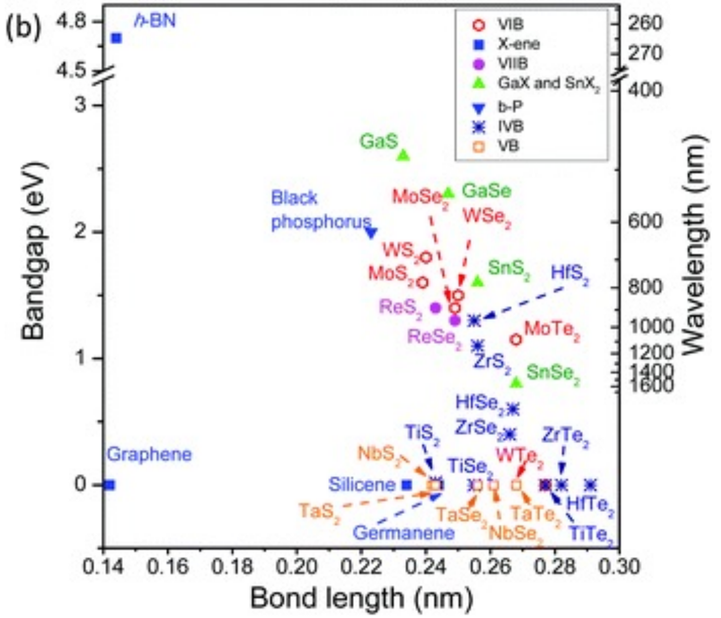
W. Choi et al., Materials Today 20 (2017), 3

MX_2 (M=Mo, W… : X=S, Se, Te)





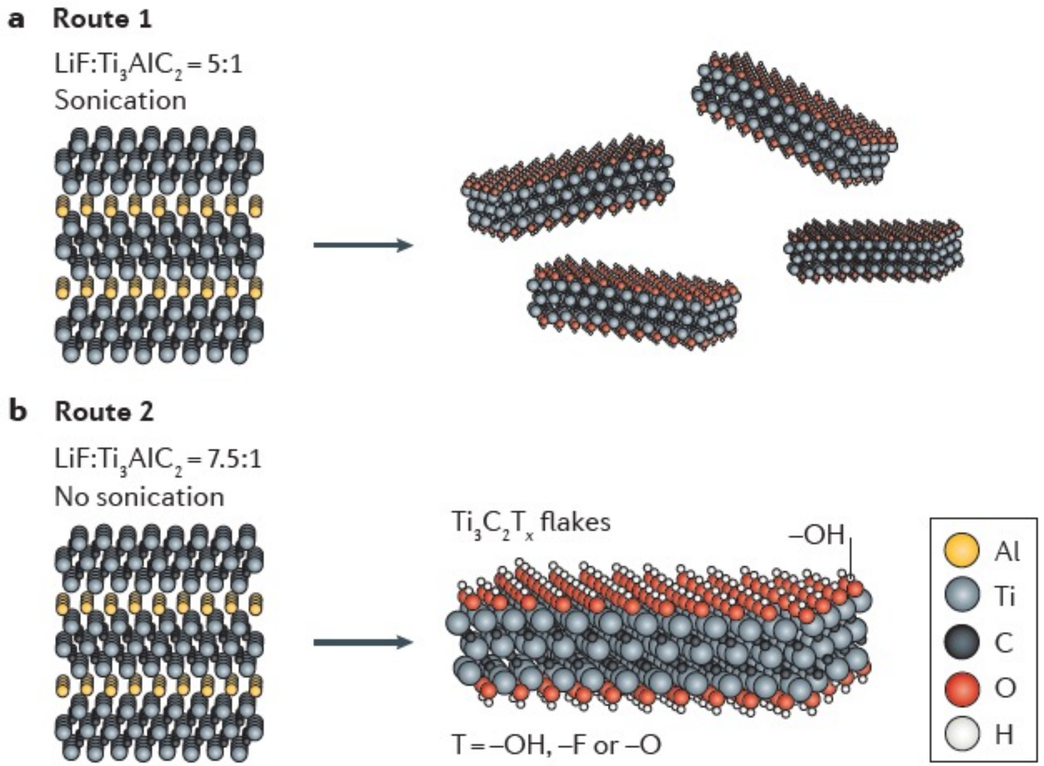
https://phys.org/news/2016-04-scientists-valleytronics-closer-reality.html

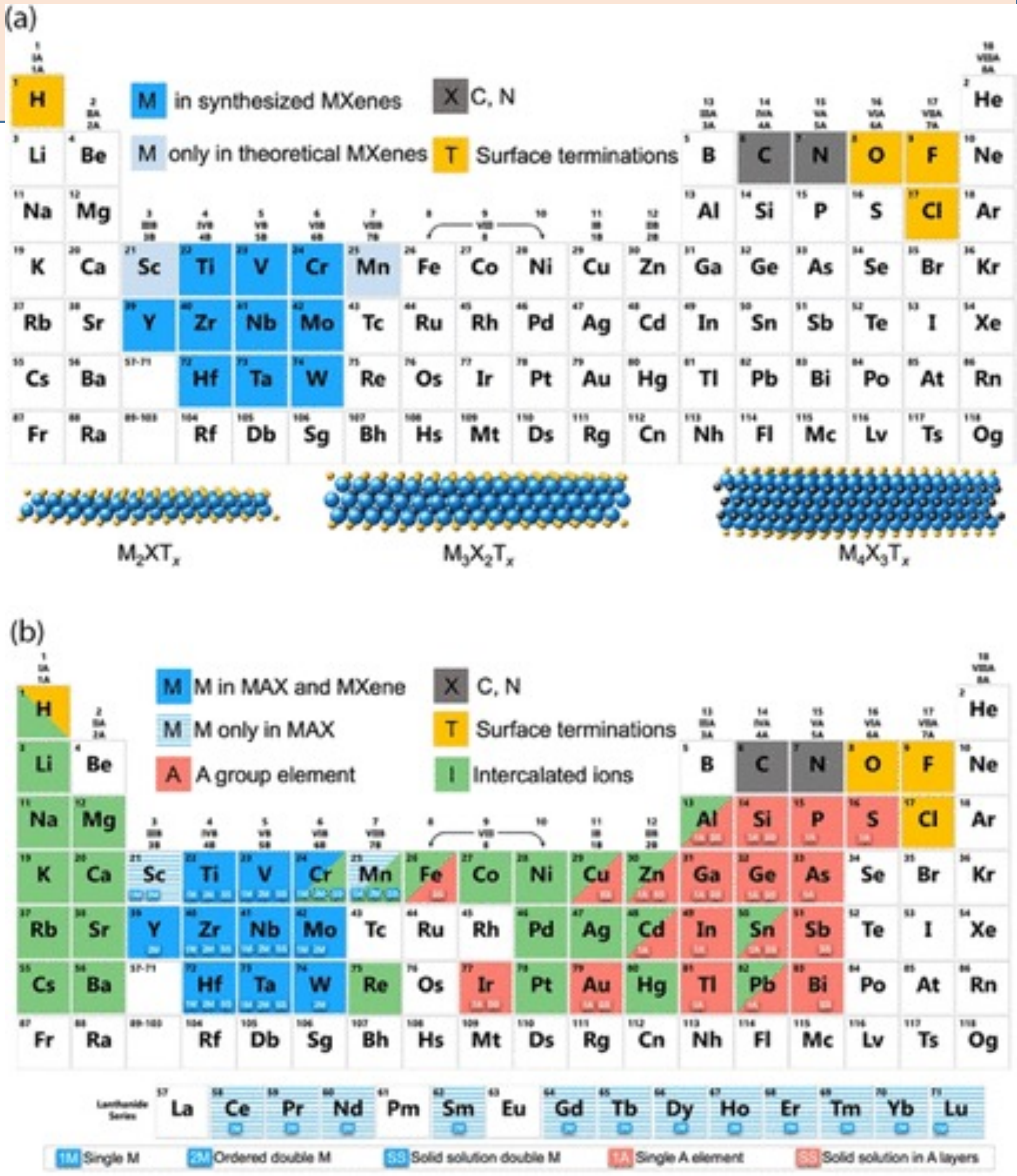


L. M. Xie, Nanoscale, 2015, 7, 18392-18401

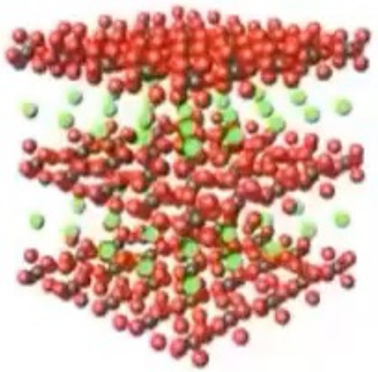
2D Materials: MXenes

- MXenes ‘$M_{n+1}X_n$’
  - Are obtained from ‘MAX’ phases by removing ‘A’ atoms
- Functionalization ‘$M_{n+1}X_nT$’
  - Surface termination groups ‘T’ emerges in production



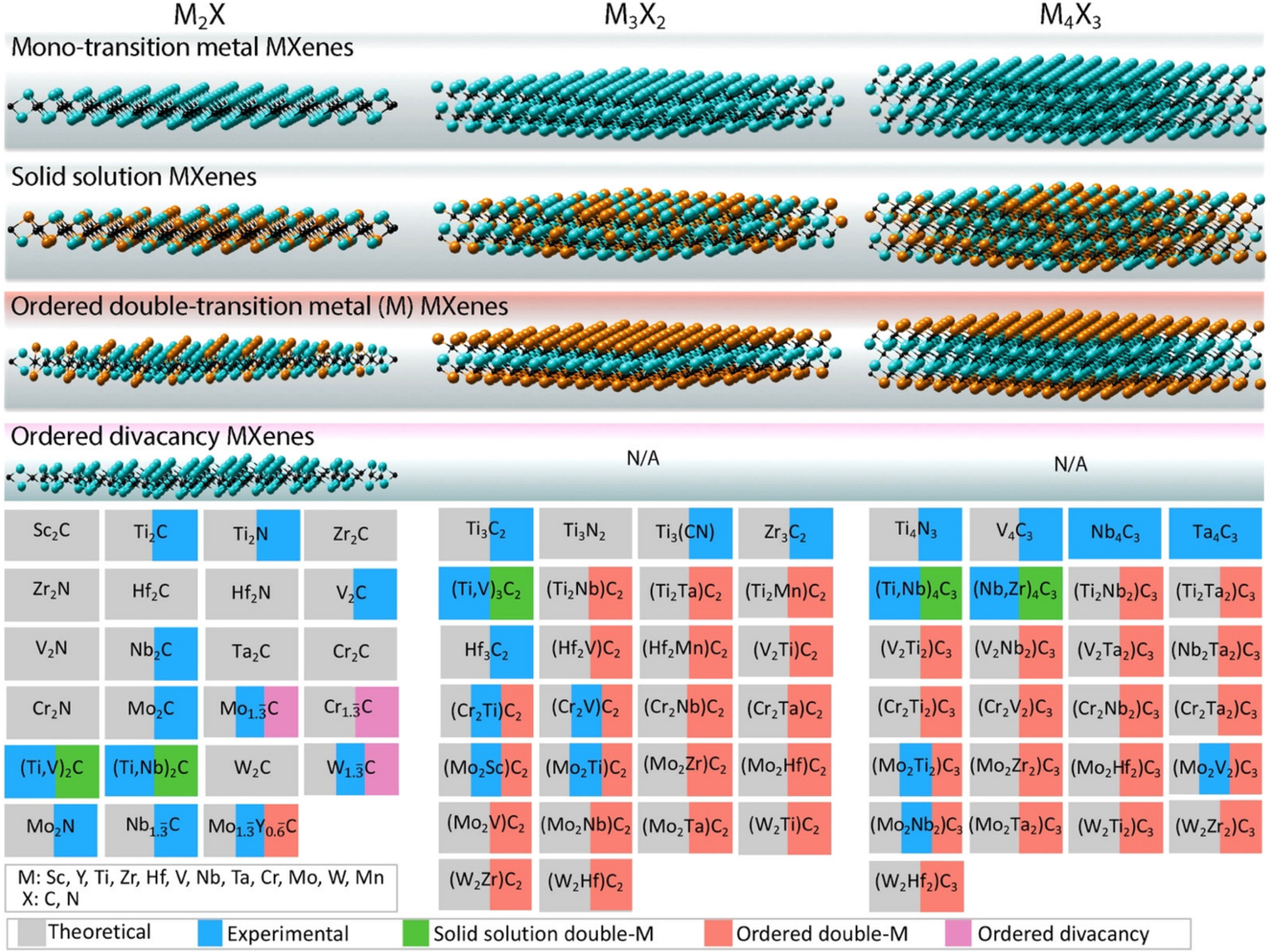


MXenes



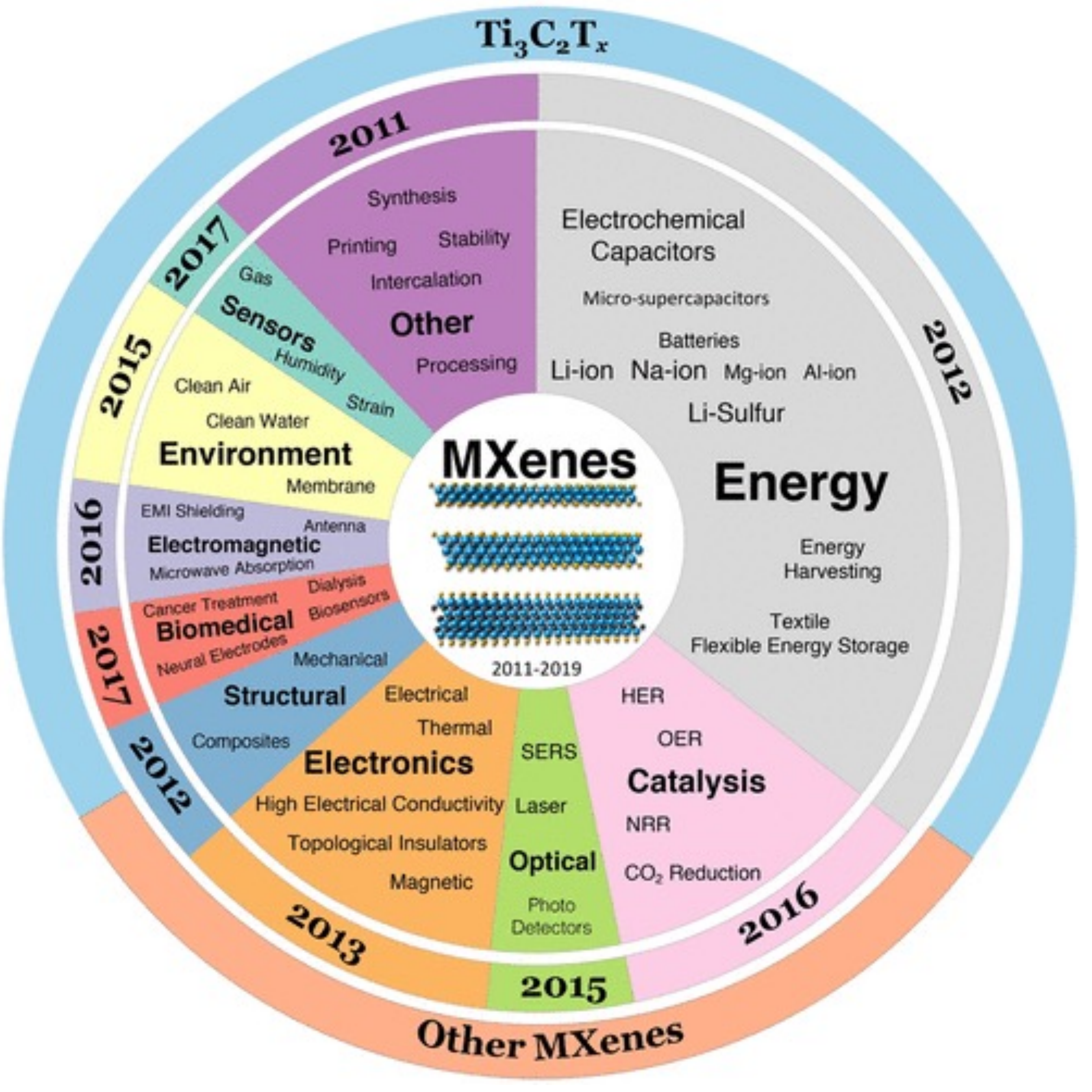
2D Materials: MXenes

- Predicted to be metallic
- Tunable properties
    - Surface terminations
    - Different metals or pairing
- combines metallic conductivity with the hydrophilic nature of termination groups
- promising for
    - Li-ion batteries
    - Supercapacitors
    - Composites
    - Photocatalysis
    - water purification
    - gas sensors



Yury Gogotsi and Babak Anasori, *ACS Nano* 2019, 13, 8, 8491–8494

2D Materials: MXenes



Y. Gogotsi, B. Anasori, *ACS Nano 13,* 2019, 8491-8494

Table 1 | **Applications of MXenes beyond energy storage**

Application	Material	Description	Refs
Structural composite	$Ti_3C_2T_x$–polyethylene, $Ti_3C_2T_x$–PVA and $Ti_3C_2T_x$–PDDA	Improved strength, hardness and creep, and anti-friction properties	117,119
Electromagnetic interference shielding	$Ti_3C_2T_x$, $Mo_2TiC_2T_x$, $Mo_2Ti_2C_3T_x$ and $Ti_3C_2T_x$–sodium alginate	MXene paper and its composite thin-filtered papers block as well as aluminium and copper, from low frequencies (30 MHz–1.5 GHz) to the X-band (8.2–12.4 GHz)	68,158, 159
Water purification	$Ti_3C_2(OH,ONa)_xF_{2-x}$	Lead adsorption	153
	TiO_2–C or TiC	Toxic heavy metal Cr(VI) adsorption	160
	$Ti_3C_2(OH)_2$	Heavy metal adsorption (for example, lead)	161
	$Ti_3C_2T_x$–iron oxide	Phosphate sequestration	162
Water desalination	$Ti_3C_2T_x$	Freestanding membranes for the charge- and size-selective rejection of ions and molecules	82,163
Nanofiltration	$Ti_3C_2T_x$–PEI or PDMS	Solvent-resistant nanofiltration for alcohol-based system	120
Dye adsorption	$Ti_3C_2T_x$	Multilayered MXene powder to adsorb methylene blue	98
Nuclear waste management	$Ti_3C_2(OH)_2$	Uranyl species adsorption	164
	V_2CT_x	Uranium (U(VI)) sorbent	165
CO_2 sensor	V_2C–PDMAEMA	Smart CO_2 and temperature sensors	166
NH_3 sensor	Ti_2CO_2	NH_3 sensor or capturer with high sensitivity and selectivity	85,167
CO catalyst	Ti-anchored Ti_2CO_2	First-principles computations on CO catalytic oxidation	168
O_2 evolution electrocatalyst	$Ti_3C_2T_x$–graphitic C_3N_4	Freestanding, binder-free flexible oxygen electrode with high activity and strong durability for rechargeable Zn–air batteries	169
H_2 generation	RuNi–$Ti_3C_2T_x$	Hydrogen generation from hydrolysis of ammonia borane	170
Ammonium perchlorate decomposition	$Ti_3C_2T_x$–Cu_2O	Thermal decomposition of ammonium perchlorate for efficient rocket propellant combustion	171
Photocatalysis	$Ti_3C_2T_x$–TiO_2	Organic contaminants decomposition and water purification	172
N_2 capture and NH_3 production	$Ti_3C_2T_x$, $V_3C_2T_x$ and $Nb_3C_2T_x$	Capturing N_2 and catalytic conversion to NH_3	173
Biosensors	$Ti_3C_2T_x$	Neural activity probe, dopamine label-free detection, monitoring spiking activity in hippocampal neuron and enzyme immobilization	155,174
Antibacterial activity	$Ti_3C_2T_x$	Resistance to biofouling against *Escherichia coli* (*E. coli*) and *Bacillus subtilis* (*B. subtilis*)	175
Photothermal therapy	$Ti_3C_2T_x$	Laser irradiation for 5 minutes increased the MXene colloid temperature above the photoablation limit of 60 °C	157
Cement hydration	$Ti_3C_2T_x$	Improving the early-age compressive strength of cement paste	176
Electronics	MXenes–TMDs	From field-effect transistors to semiconductors with tunable bandgaps	61,77, 80,106
Lubrication	$Ti_3C_2T_x$	Lubrication additive in base oil	156,177

Nature Reviews Materials **2**, Article number: 16098 (2017)

2D Materials: MXenes

Published: 06 November 2012

Electronics and optoelectronics of two-dimensional transition metal dichalcogenides

Qing Hua Wang, Kourosh Kalantar-Zadeh, Andras Kis, Jonathan N. Coleman & Michael S. Strano

Nature Nanotechnology 7, 699–712 (2012) | Cite this article

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Progress Report | Full Access

25th Anniversary Article: MXenes: A New Family of Two-Dimensional Materials

Michael Naguib, Vadym N. Mochalin, Michel W. Barsoum, Yury Gogotsi

First published: 19 December 2013 | https://doi.org/10.1002/adma.201304138 | Citations: 2,704

Published: 13 June 2017

2D transition metal dichalcogenides

Sajedeh Manzeli, Dmitry Ovchinnikov, Diego Pasquier, Oleg V. Yazyev & Andras Kis

Nature Reviews Materials 2, Article number: 17033 (2017) | Cite this article

IOP Publishing
Nanotechnology 27 (2016) 335702 (10pp) doi:10

Vibrational and mechanical properties of single layer MXene structures: a first-principles investigation

Uğur Yorulmaz[1], Ayberk Özden[1], Nihan K Perkgöz[2], Feridun Ay[2] and Cem Sevik[3]

The Rise of MXenes

Yury Gogotsi* and Babak Anasori*

Cite this: *ACS Nano* 2019, 13, 8, 8491–8494
Publication Date: August 27, 2019
https://doi.org/10.1021/acsnano.9b06394

Cite this: *Nanoscale*, 2020, **12**, 17354

First-principles exploration of superconductivity in MXenes†

Jonas Bekaert, *‡[a] Cem Sevik ‡[b] and Milorad V. Milošević [a]

Cite this: *J. Mater. Chem. A*, 2018, **6**, 2337

MXenes/graphene heterostructures for Li battery applications: a first principles study†

Yierpan Aierken,[a] Cem Sevik,[b] Oğuz Gülseren,[c] François M. Peeters[a] and Deniz Çakır *[ad]

Cite this: *Nanoscale*, 2018, **10**, 8859

The influence of surface functionalization on thermal transport and thermoelectric properties of MXene monolayers†

Sevil Sarikurt, *[a] Deniz Çakır, *[b] Murat Keçeli *[c] and Cem Sevik *[d]

Cite this: *J. Mater. Chem. A*, 2020, **8**, 19674

High-throughput computational screening of 2D materials for thermoelectrics†

Sevil Sarikurt, *[ab] Tuğbey Kocabaş [c] and Cem Sevik *[b]

ADVANCED MATERIALS

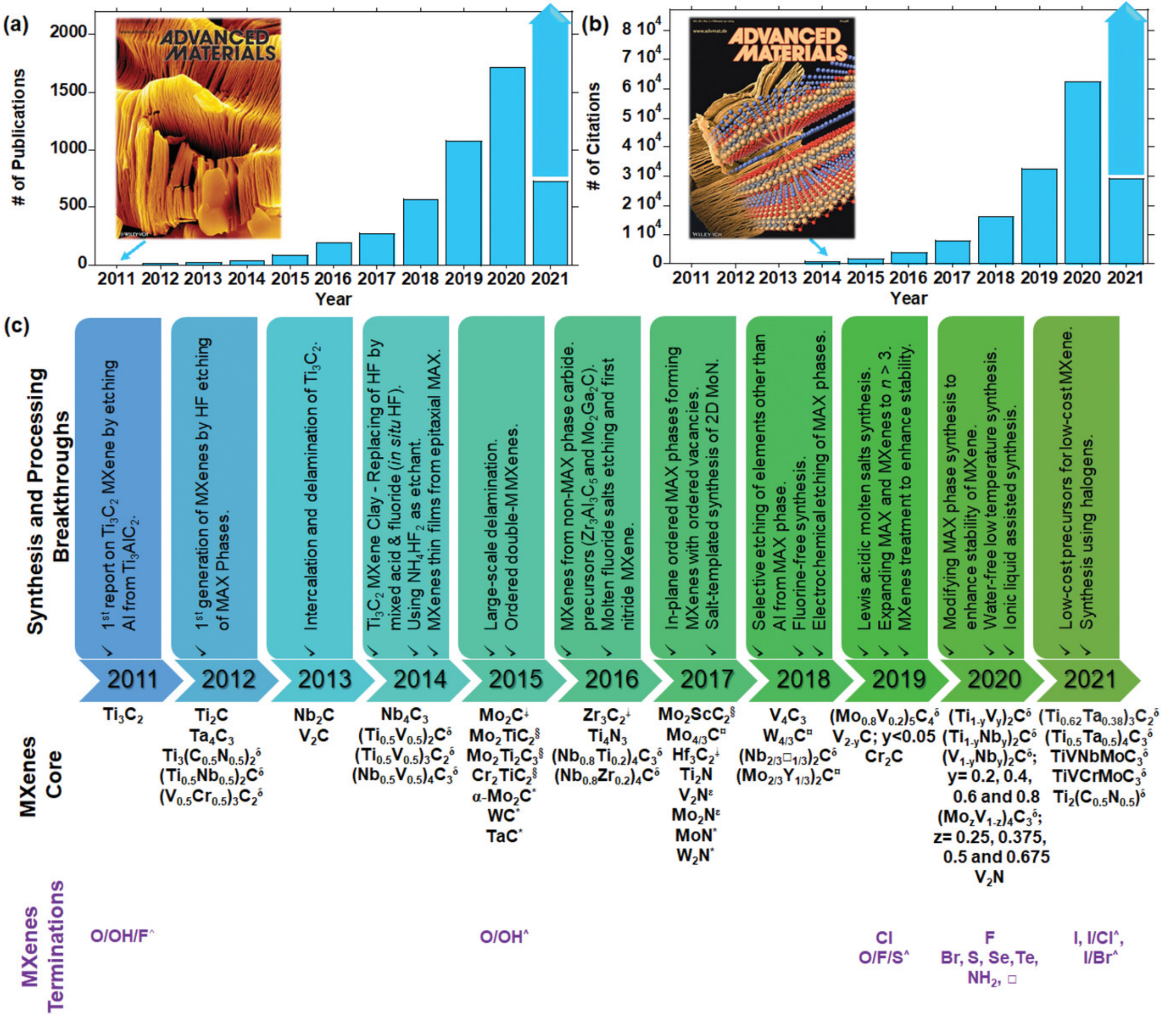
Advanced Materials homepage

Perspective | Full Access

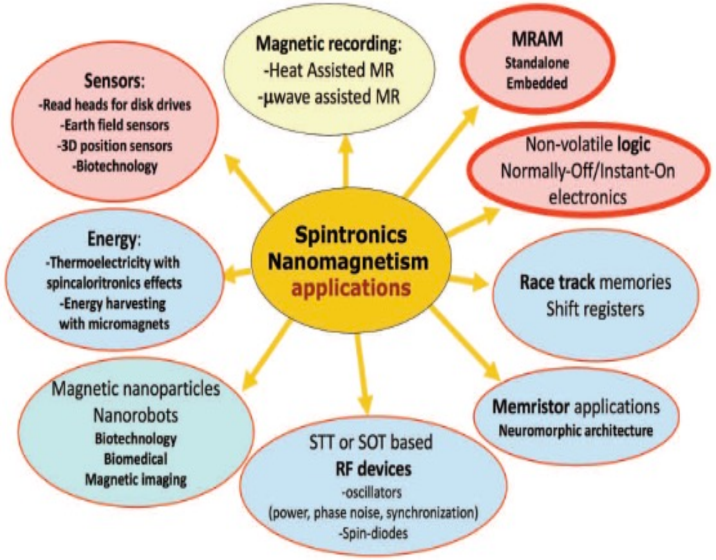
Ten Years of Progress in the Synthesis and Development of MXenes

Michael Naguib, Michel W. Barsoum, Yury Gogotsi

First published: 16 August 2021 | https://doi.org/10.1002/adma.202103393 | Citations: 1



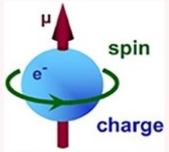
2D Materials - Magnetism



Zhang, W., et al. (2019)
InfoMat, 1(4), 479-495.

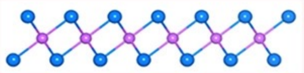
2D Spintronics

Charge spins



+

2D materials



Challenges & Opportunities

- **Scalability**
- **Ambient stability**
- **Curie temperatures**
- **Interface-induced magnetic phenomena:** half-metallicity at Co/MoS_2 interface, giant magnetoresistance in vertical $Fe/MoS_2/Fe$ junction, PMA at $CoFeB/MoSe_2$ interface, interface magnetic proximity, spin-orbit torque, spin pumping, multiferroicity, 2D spin-liquids, skymions…

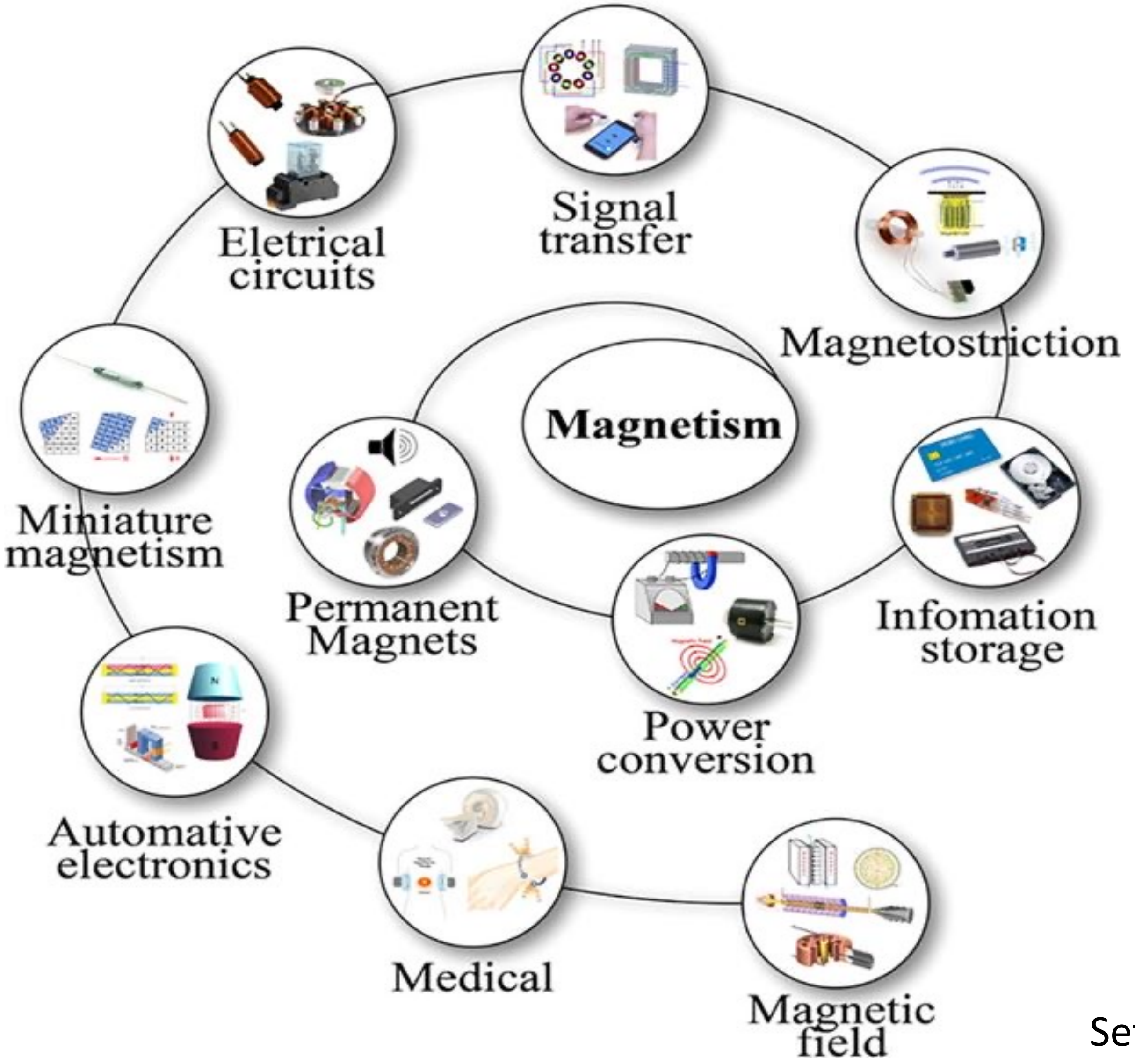
2D-vdW Magnets

- **Extrinsic magnetism:** defect engineering, surface functionalization, doping
- **Intrinsic magnetism:** CrX_3 (X = Cl, Br and I), $CrGeTe_3$, Fe_3GeTe_2, MnX_2 (X = S, Se), VX_2 (X = S, Se, Te), and 2D oxides, halides, nitrides, carbides…
- **Devices:** vdW-MTJs…

Advances in Growth & Characterization Techniques

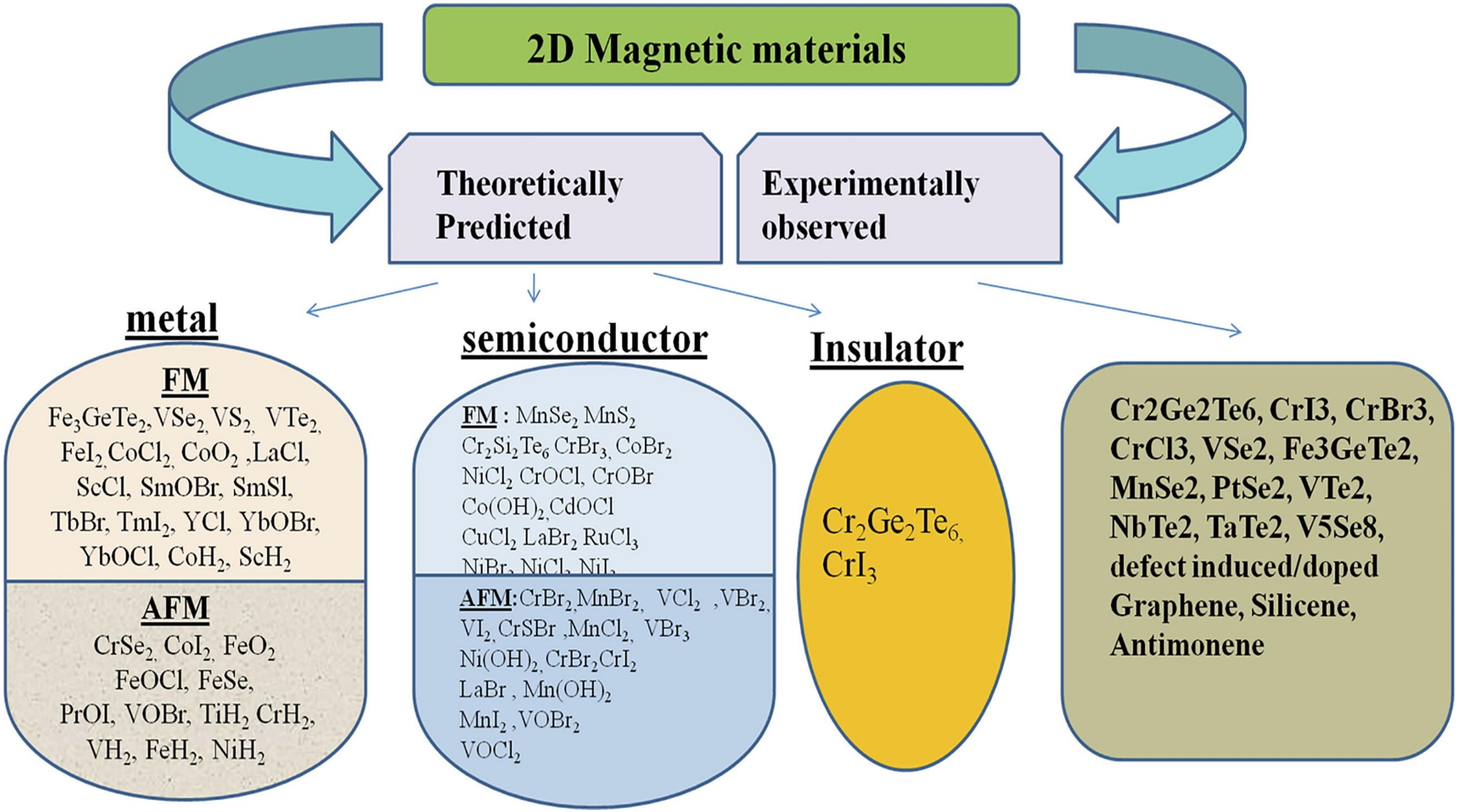
- **Specialized growth techniques:** gas-assisted MBE, plasma-assisted MBE…
- **Nanoscale magnetic characterization tools:** scanning single-spin magnetometry…

Applications of Magnetism



Sethulakshmi, N. et al. *Materials Today* 27 (2019): 107-122.

2D Magnetic Materials



Bagga, V., & Kaur, D. (2020). Materials Today: Proceedings, 28, 1938-1942.

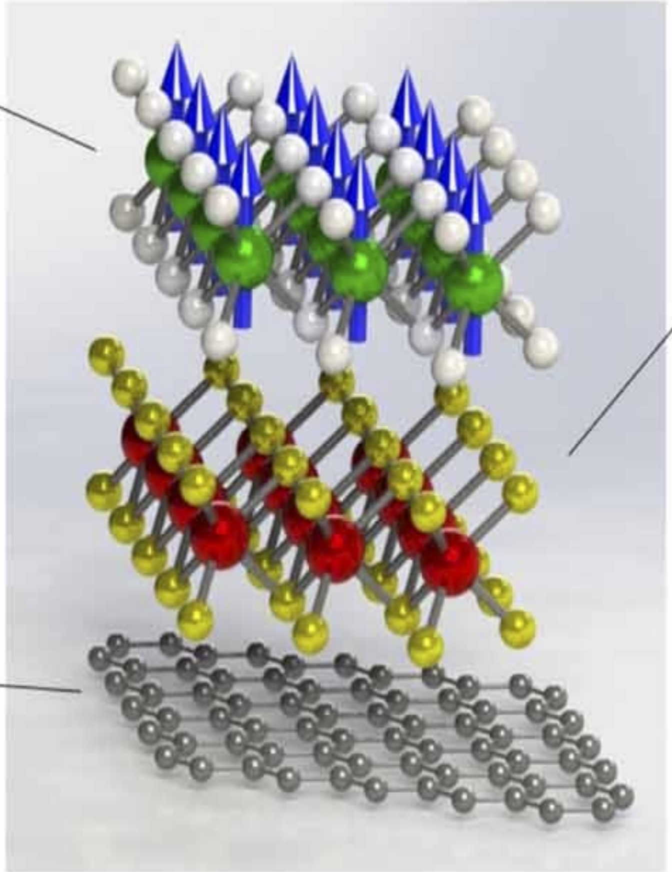
Spin and Magnetism in 2D Materials

2D magnets

Non-volatile storage
Spin filtering
Spin injection and detection

Transition metal dichalcogenides

Strong spin-orbit coupling
Valley optical selection rules
Quantum spin Hall effect

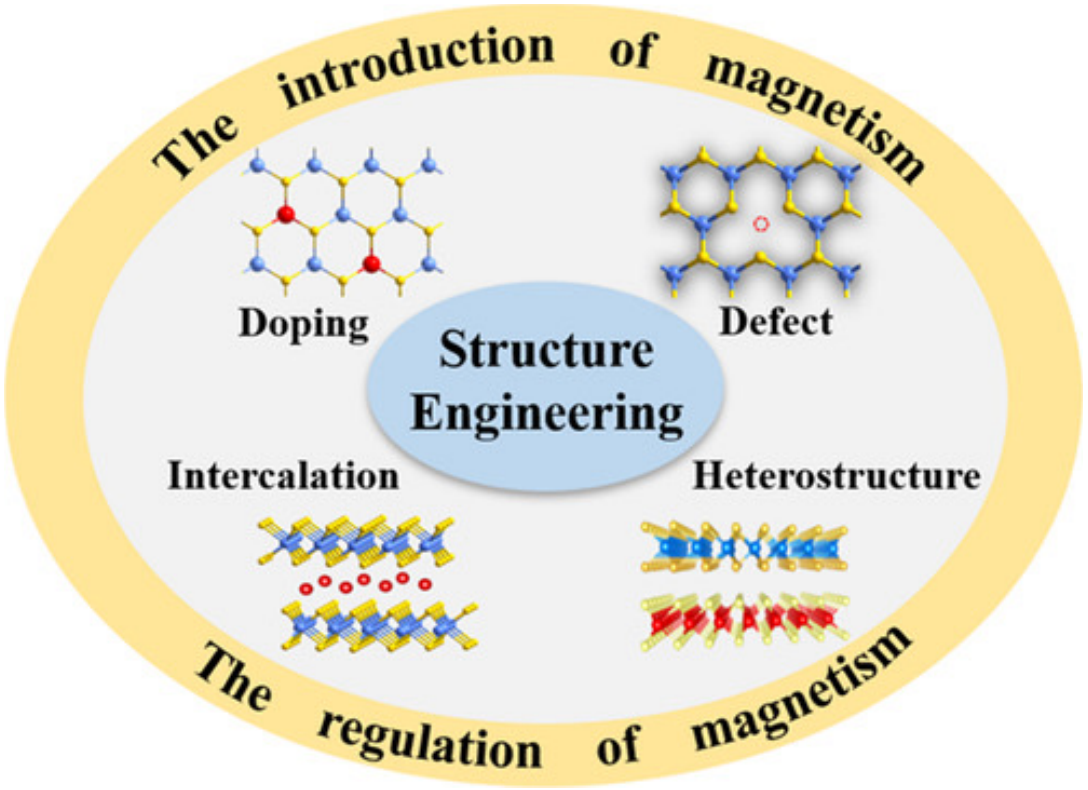


Graphene

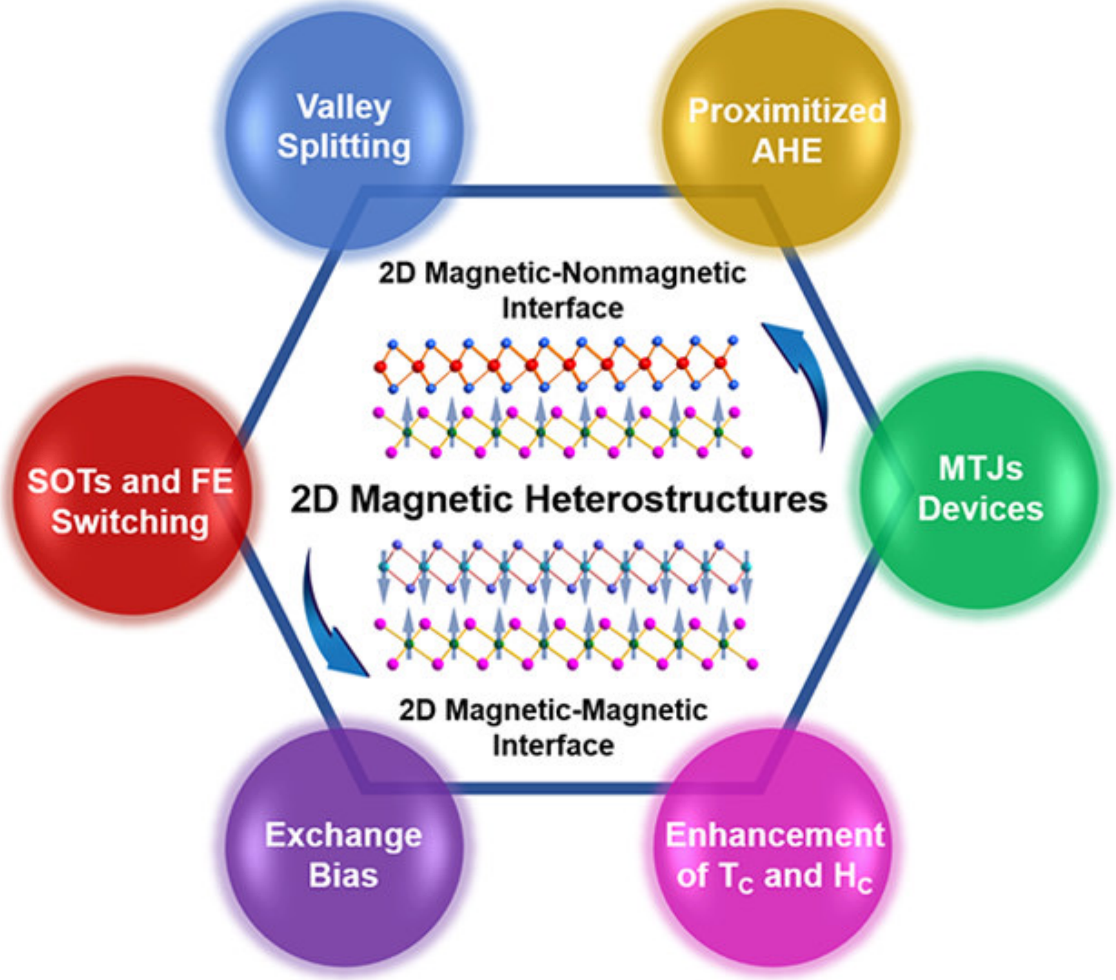
Long spin diffusion lengths
Dirac dispersion
Weak spin-orbit coupling

Vedmedenko, E. Y. et al (2020). Journal of Physics D: Applied Physics, 53(45), 453001.

2D Magnetic Materials



Zhao, Z. et al. (2021) *Small Structures*, *2*(10), 2100077.



Wei Li et al., *ACS Appl. Mater. Interfaces* 2021, 13, 43, 50591–50601

2D Magnetic Materials

Published: 26 April 2017

Discovery of intrinsic ferromagnetism in two-dimensional van der Waals crystals

Cheng Gong, Lin Li, Zhenglu Li, Huiwen Ji, Alex Stern, Yang Xia, Ting Cao, Wei Bao, Chenzhe Wang, Yuan Wang, Z. Q. Qiu, R. J. Cava, Steven G. Louie, Jing Xia & Xiang Zhang

Nature **546**, 265–269 (2017) | Cite this article

Published: 08 June 2017

Layer-dependent ferromagnetism in a van der Waals crystal down to the monolayer limit

Bevin Huang, Genevieve Clark, Efrén Navarro-Moratalla, Dahlia R. Klein, Ran Cheng, Kyle L. Seyler, Ding Zhong, Emma Schmidgall, Michael A. McGuire, David H. Cobden, Wang Yao, Di Xiao, Pablo Jarillo-Herrero & Xiaodong Xu

Nature **546**, 270–273 (2017) | Cite this article

Review Article | Published: 27 September 2019

Probing and controlling magnetic states in 2D layered magnetic materials

Kin Fai Mak, Jie Shan & Daniel C. Ralph

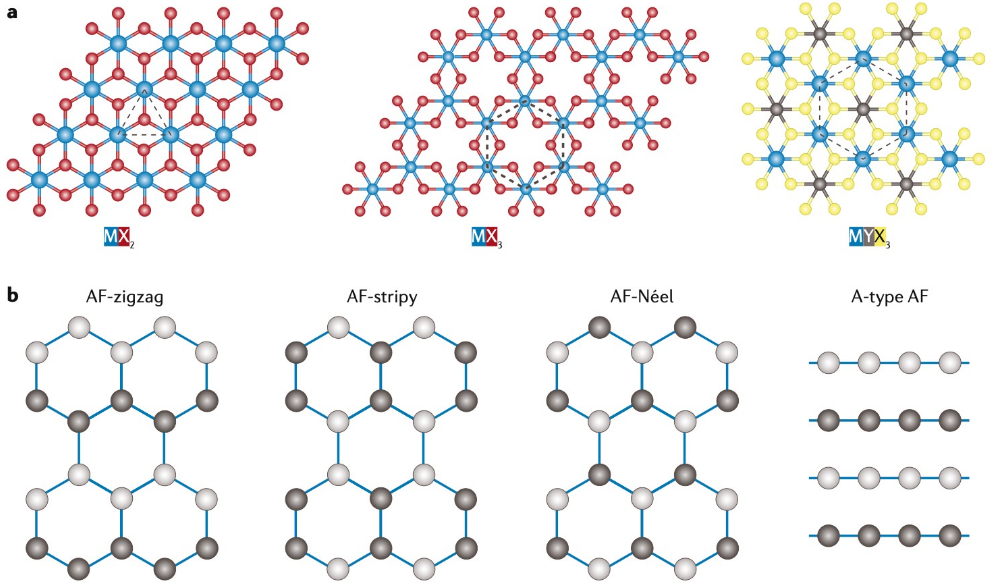
Nature Reviews Physics **1**, 646–661 (2019) | Cite this article

Review Article | Published: 07 May 2019

Magnetic 2D materials and heterostructures

M. Gibertini, M. Koperski, A. F. Morpurgo & K. S. Novoselov

Nature Nanotechnology **14**, 408–419 (2019) | Cite this article



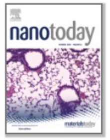
REVIEW SUMMARY

MAGNETISM

Two-dimensional magnetic crystals and emergent heterostructure devices

Cheng Gong and Xiang Zhang*

2D Magnetic Materials



nanotoday
Volume 34, October 2020, 100902

Recent breakthroughs in two-dimensional van der Waals magnetic materials and emerging applications

Yahya Khan [a], Sk. Md. Obaidulla [a], Mohammad Rezwan Habib [a], Anabil Gayen [a], Tao Liang [a], Xuefeng Wang [b], Mingsheng Xu [a, c]

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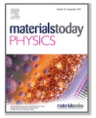
2D Magnetic Heterostructures and Their Interface Modulated Magnetism

Wei Li, Yi Zeng, Zijing Zhao, Biao Zhang, Junjie Xu, Xiaoxiao Huang, and Yanglong Hou*

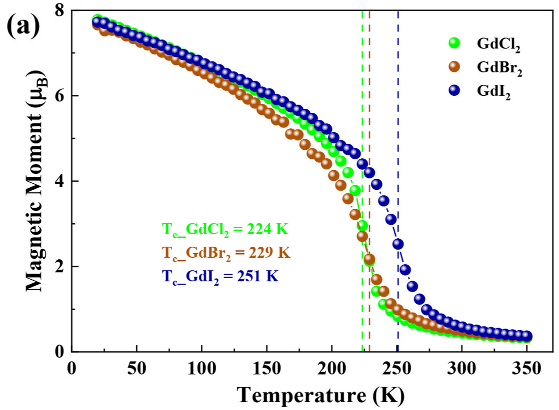
Cite this: *ACS Appl. Mater. Interfaces* 2021, 13, 43, 50591–50601
Publication Date: October 21, 2021
https://doi.org/10.1021/acsami.1c11132



ELSEVIER
Materials Today Physics
Volume 21, November 2021, 100514

Two-dimensional ferromagnetic semiconductors of rare-earth monolayer GdX_2 (X = Cl, Br, I) with large perpendicular magnetic anisotropy and high Curie temperature

Weiqi Liu [a], Junwei Tong [a], Li Deng [a], Bo Yang [a], Guangming Xie [b], Gaowu Qin [a], Fubo Tian [c], Xianmin Zhang [a]



DOI: 10.1039/D0NR06813F (Review Article) *Nanoscale*, 2021, **13**, 1398-1424

Two-dimensional magnetic materials: structures, properties and external controls

Shuqing Zhang [ab], Runzhang Xu [a], Nannan Luo [c] and Xiaolong Zou [*a]

small structures
Review | Free Access

Structure Engineering of 2D Materials toward Magnetism Modulation

Zijing Zhao, Wei Li, Yi Zeng, Xiaoxiao Huang, Chao Yun, Biao Zhang, Yanglong Hou

First published: 27 August 2021 | https://doi.org/10.1002/sstr.202100077

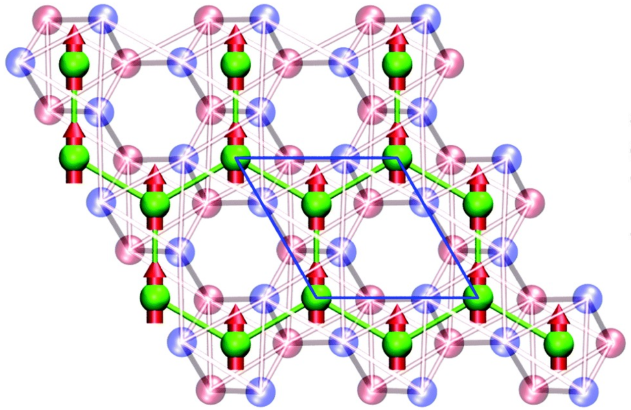
2D Magnetic Materials: CrI_3

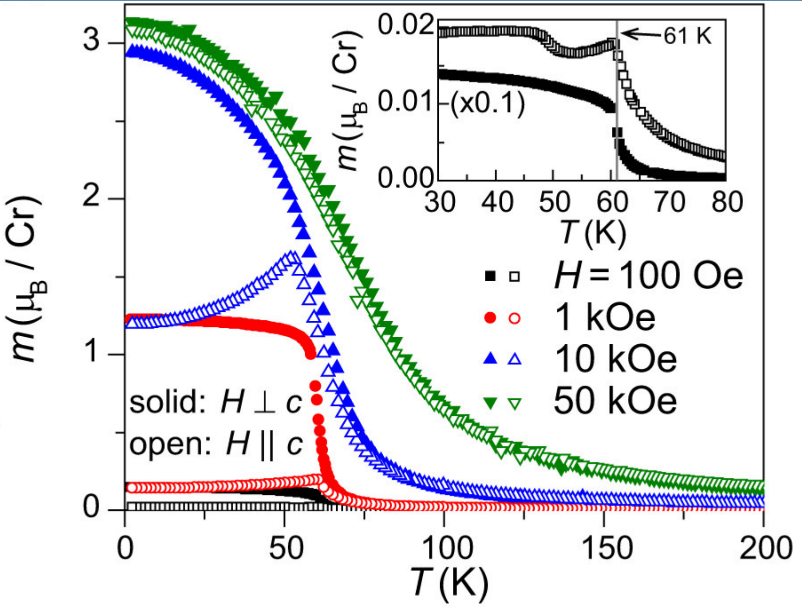
Coupling of Crystal Structure and Magnetism in the Layered, Ferromagnetic Insulator CrI_3

Michael A. McGuire*, Hemant Dixit, Valentino R. Cooper, and Brian C. Sales

View Author Information

Cite this: *Chem. Mater.* 2015, 27, 2, 612–620
Publication Date: December 23, 2014
https://doi.org/10.1021/cm504242t





Cite this: *J. Mater. Chem. C*, 2015, 3, 12457

Robust intrinsic ferromagnetism and half semiconductivity in stable two-dimensional single-layer chromium trihalides

Wei-Bing Zhang,*[ab] Qian Qu,[a] Peng Zhu[a] and Chi-Hang Lam*[b]

Table 4 The exchange coupling and Curie temperature of single-layer chromium trihalides

	J_{NN}^{HSE06} meV	J_{NN} meV	J_1 meV	J_2 meV	J_3 meV	T_C^{NN} K	T_C K
CrF_3	0.8688	1.7904	1.8028	0.0672	−0.0128	36	41
$CrCl_3$	1.8728	1.7908	1.9232	0.2264	−0.1328	36	49
$CrBr_3$	2.4216	2.4524	2.5988	0.3800	−0.1464	51	73
CrI_3	3.3216	2.7096	2.8624	0.6384	−0.1532	56	95

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Bevin Huang, Genevieve Clark, Efrén Navarro-Moratalla, Dahlia R. Klein, Ran Cheng, Kyle L. Seyler, Ding Zhong, Emma Schmidgall, Michael A. McGuire, David H. Cobden, Wang Yao, Di Xiao, Pablo Jarillo-Herrero & Xiaodong Xu

Nature **546**, 270–273 (2017) | Cite this article

On the origin of magnetic anisotropy in two dimensional CrI_3

J L Lado[1] and J Fernández-Rossier[1,2]

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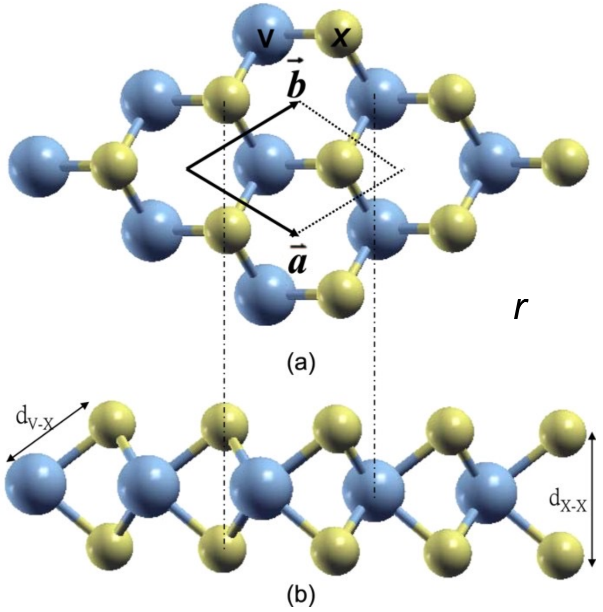
2D Materials, Volume 4, Number 3
Citation J L Lado and J Fernández-Rossier 2017 *2D Mater.* **4** 035002

V-based van der Waals Magnets: VX_2(X=S, Se, Te)



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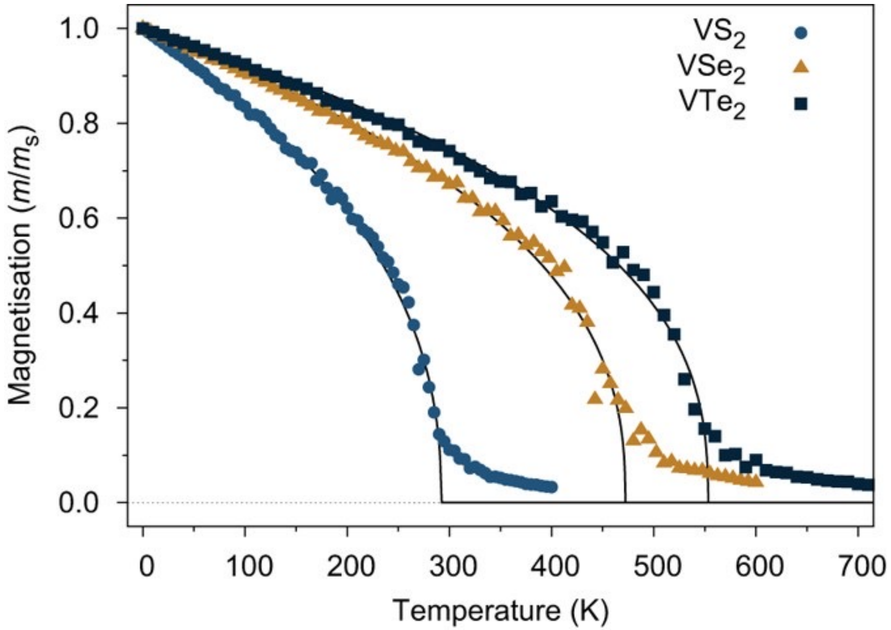
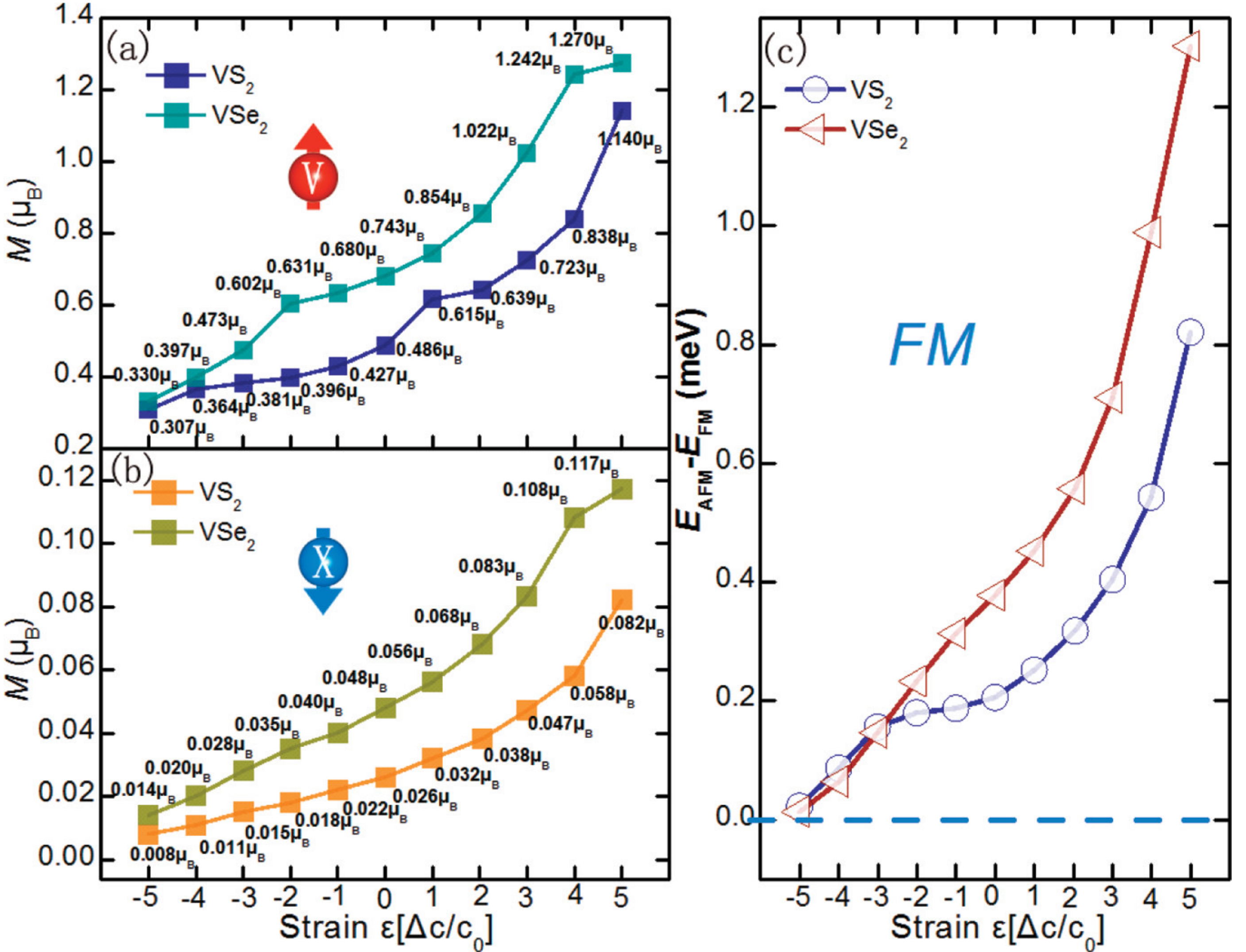


Zhang H. et al. J. Mater. Chem. A, 2013,1, 10821-10828



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TÜBİTAK ULAKBİM

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