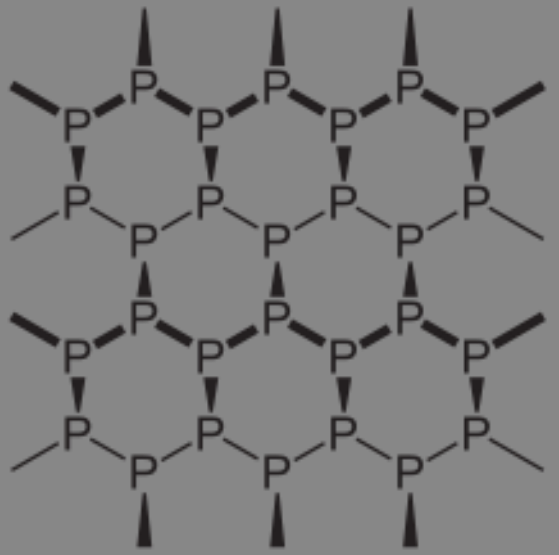
UNIVERSITÄT LEIPZIG

AUS TRADITION
GRENZEN ÜBERSCHREITEN

Two-dimensional crystals containing phosphorus

Thomas Heine

Wilhelm-Ostwald-Institut für
Physikalische und Theoretische Chemie



Disclaimer:

This presentation is not on black phosphorus (resp. phosphorene)!

Liquid Exfoliation of Layered Materials

Valeria Nicolosi, Manish Chhowalla, Mercouri G. Kanatzidis, Michael S. Strano, Jonathan N. Coleman*

READ THE FULL ARTICLE ONLINE
http://dx.doi.org/10.1126/science.1226419

Cite this article as V. Nicolosi *et al.*, *Science* **340**, 1226419 (2013). DOI: 10.1126/science.1226419

Mayan blue (400 CE):

- Mixture of indigo (organic dye) and palygorskite (layered clay)
- Exfoliation of clay by heating
- Mayan blue is greenish, due to blue indigo and yellowish exfoliated clays
- This was possibly the first human application of quantum confinement

Definition of Layered Material:

- Strong, directed intralayer bonds (covalent, partially ionic), weak undirected interlayer bonds (London dispersion, ionic)

Definition two-dimensional (2D) material

- Single (1L) or few (nL) layers of a layered material

There is a plethora of natural layered materials!

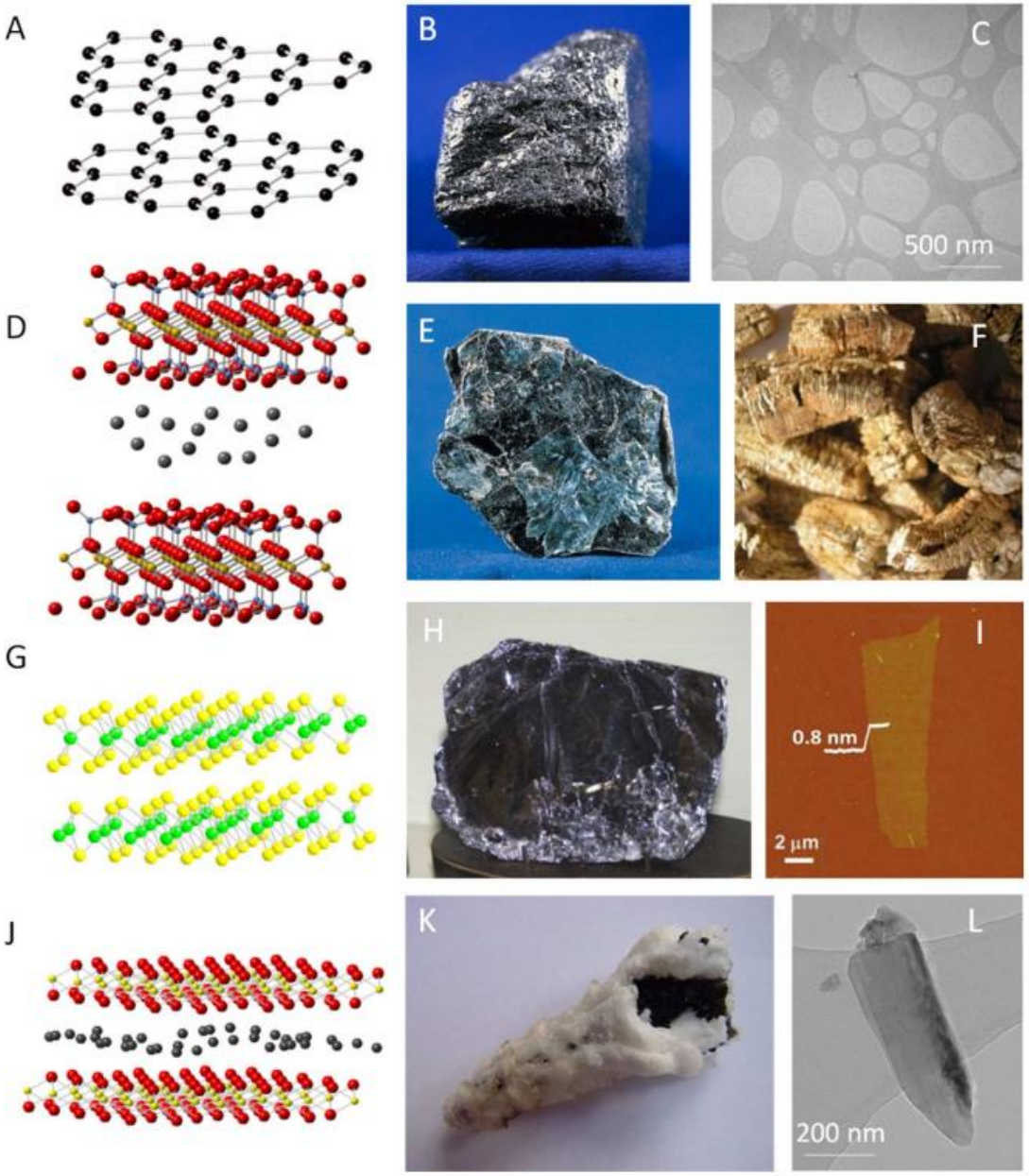
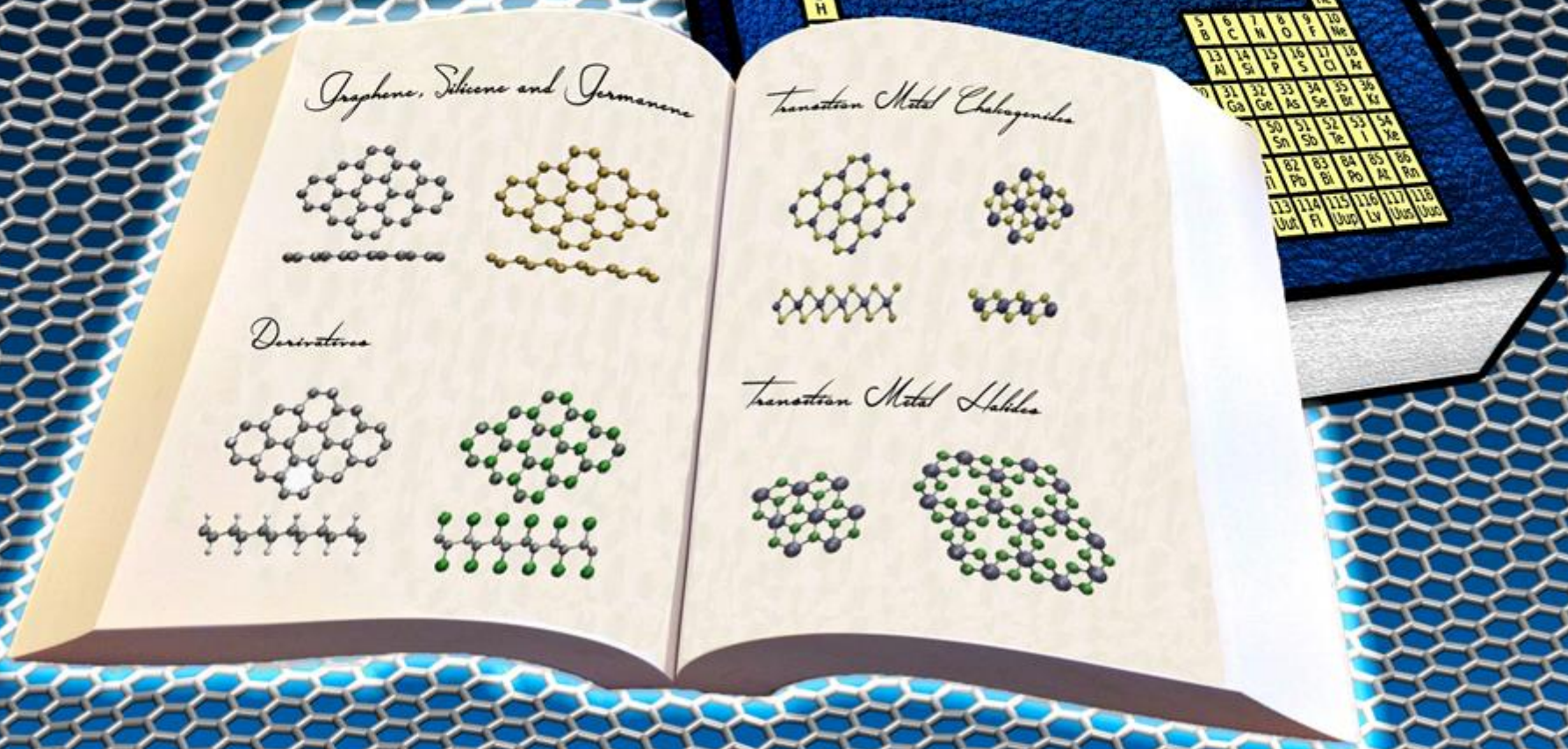


Fig. 1. Crystal structures, naturally occurring forms, and exfoliated products for four example layered materials. (**A**) Graphite consists of alternating stacks of hexagonally arranged carbon atoms (black spheres), (**B**) is a naturally occurring mineral, and (**C**) exfoliates to single atomic layers of carbon called graphene. (**D**) Vermiculite is a layered silicate hydrate (typically $Mg_{1.8}Fe_{0.9}Al_{4.3}SiO_{10}(OH)_2{\cdot}4(H_2O)$ that (**E**) is found naturally as a mineral and (**F**) can be exfoliated, for example, upon heating. Silicon atoms are in blue, oxygen atoms are in red, Al/Mg/Fe atoms are in yellow, and interlayer counterions are in black (H and H_2O not shown). (**G**) MoS_2 is a layered arrangement of S and Mo atoms (chalcogen atoms are in yellow, and transition metal are in green) that (**H**) is found naturally as the mineral molybdenite and (**I**) can be exfoliated to MoS_2 monolayers. (**J**) Layered manganese dioxide (manganese atoms are in yellow, oxygen is in red, and interlayer counterions are in black) occurs naturally (**K**) as birnessite and (**L**) can be exfoliated to give MnO_2 nanosheets. (C), (I), and (L) are adapted from (*48*), (*87*), and (*58*), respectively. The layer spacings for each material are graphite, 0.35 nm; vermiculite, 1.5 nm; MoS_2, 0.6 nm; and MnO_2, 0.45 nm.

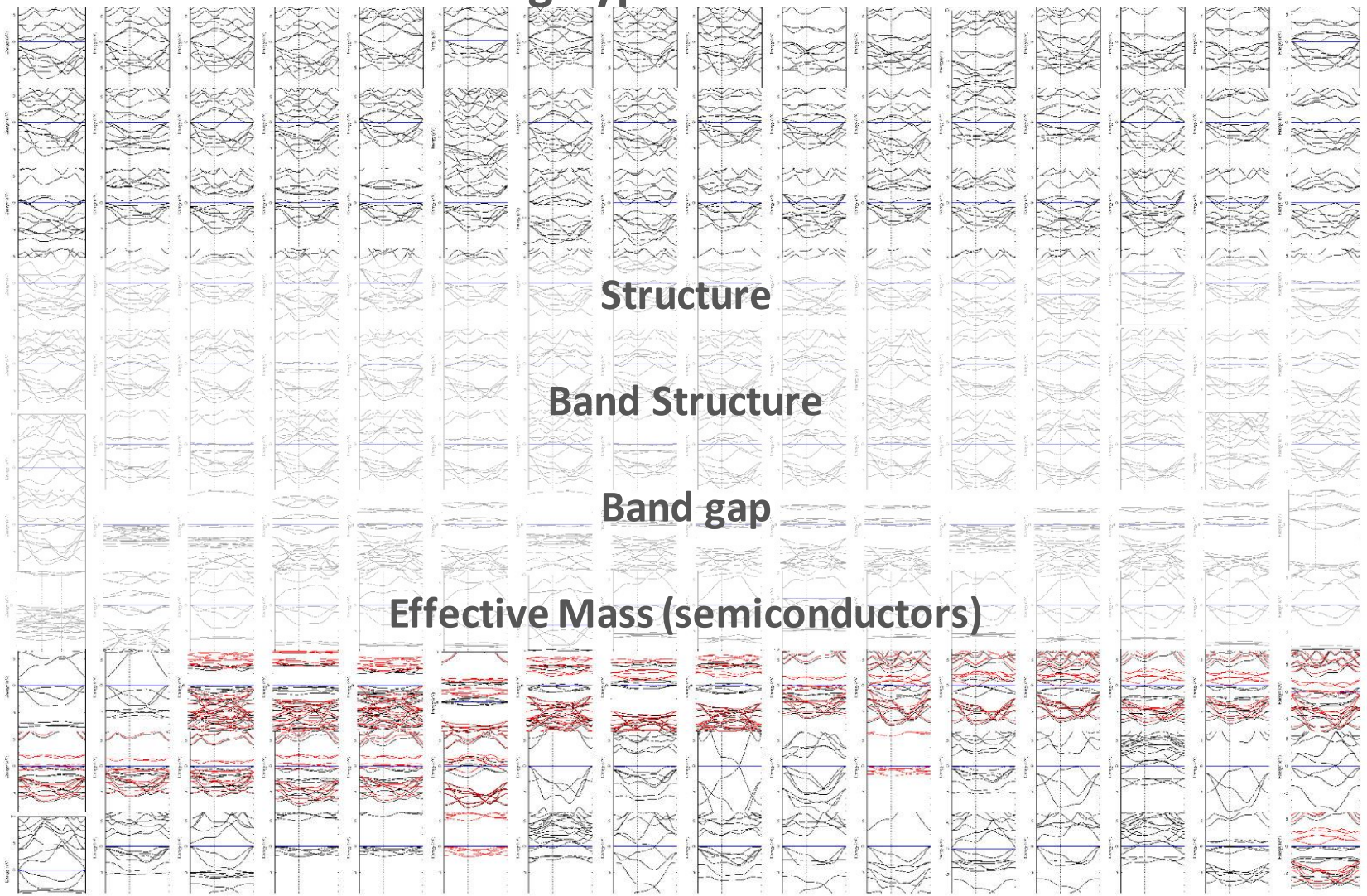
V. Nicolosi, M. Chhowalla, M. G. Kanatzidis, M. S. Strano, J. N. Coleman, Science 340 (2013) 1420.

P. Miró, M. Audiffred, T. Heine, Chem. Soc. Rev. 43 (2014) 6537-6554.

An Atlas of Two-Dimensional Materials



This review include more than 150 single layered materials. Including hypothetical ones.



P. Miro, M. Audiffred, T. Heine, Chem. Soc. Rev. 43 (2014) 6537-6554.

Our revised approach

- Read the (old) literature of synthetic layered materials
- Idea: quantum confinement will alter electronic properties, in particular the band gap will increase
- Identify interesting candidates, for which we investigate the exfoliated 2D crystal (in silico) in terms of
  - Stability (phonons, simulated annealing)
  - Exfoliation possibility (cleavage energy)
  - Electronic properties (band structure, charge carrier mobilities)
  - Photocatalysis and photovoltaics (absorption, band edges)
  - Electromechanical properties

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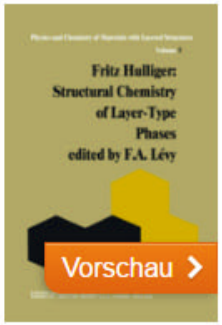
Physics and Chemistry of Materials with A



© 1976

Structural Chemistry of Layer-Type Phases

Autoren: **Hulliger**, F.
Herausgeber: **Lévy**, Francis (Ed.)

Über dieses Buch

This monograph is intended to give the reader an appreciation of the wealth of phases, elements and inorganic compounds, which crystallize in layer-type or two dimensional structures. Originally this work was planned as a short review article but the large number of phases made it grow out to the size of a book. As is evident from the arrangement of the chapters our point of view was gradually transmuting from geometric to chemical. Moreover, the decision about the compounds that should be discussed was taken only during the course of the work, as is partly evident from the

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Zahlen und Fakten

GeP_3 – better than phosphorene?

Yu Jing, Yandong Ma, Yafei Li, Thomas Heine

NanoLetters 17 (2017) 1833–1838

2D Phosphorus Carbide ?

NANO LETTERS

Letter

pubs.acs.org/NanoLett

Two-Dimensional Phosphorus Carbide: Competition between sp^2 and sp^3 Bonding

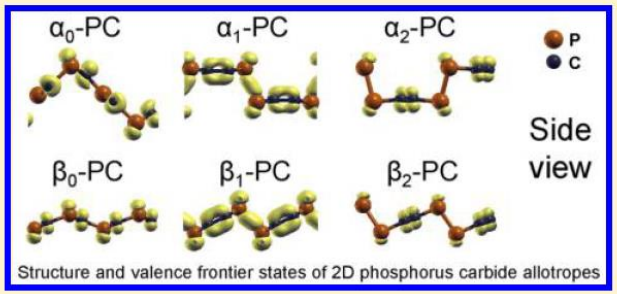
Jie Guan,[†] Dan Liu,[†] Zhen Zhu,[†,‡] and David Tománek*[,†]

[†]Physics and Astronomy Department, Michigan State University, East Lansing, Michigan 48824, United States

[‡]Materials Department, University of California, Santa Barbara, California 93106, United States

Supporting Information

ABSTRACT: We propose previously unknown allotropes of phosphorus carbide (PC) in the stable shape of an atomically thin layer. Different stable geometries, which result from the competition between sp^2 bonding found in graphitic C and sp^3 bonding found in black P, may be mapped onto 2D tiling patterns that simplify categorizing of the structures. Depending on the category, we identify 2D-PC structures that can be metallic, semimetallic with an anisotropic Dirac cone, or direct-gap semiconductors with their gap tunable by in-layer strain.



Structure and valence frontier states of 2D phosphorus carbide allotropes

Bandgap ~0.7 eV

Nano Lett. 2016, 16, 3247−3252

No solid states that consist of P and C have been found in experiment (yet)

JOURNAL OF SOLID STATE CHEMISTRY 5, 441–445 (1972)

The Crystal Structure of SnP_3 and a Note on the Crystal Structure of GeP_3

JAN GULLMAN AND OLLE OLOFSSON

Institute of Chemistry, University of Uppsala, Box

Received April 3, 1972

SnP_3 crystallizes in the trigonal space group $R\bar{3}m$ with six for
$a = 7.378$ Å and $c = 10.512$ Å. The detailed atomic arrangement
sional single crystal X ray data.

The structure is characterized as a layer structure related to t
layers consist of puckered P_6 rings connected by Sn atoms. The c
Sn atoms of adjacent layers. This leads to a distorted octahed
three phosphorus atoms belonging to the same layer as the tin
phosphorus atoms in an adjacent layer at a distance of 2.925 Å
is 2.222 Å and the P–P–P bond angle is 99.1°.

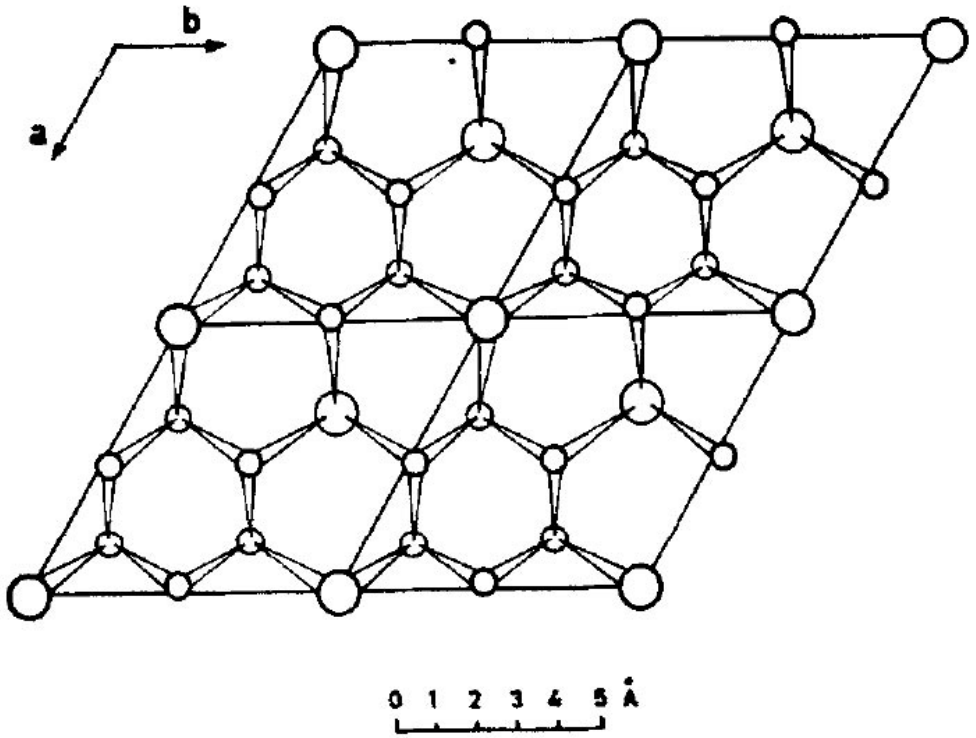
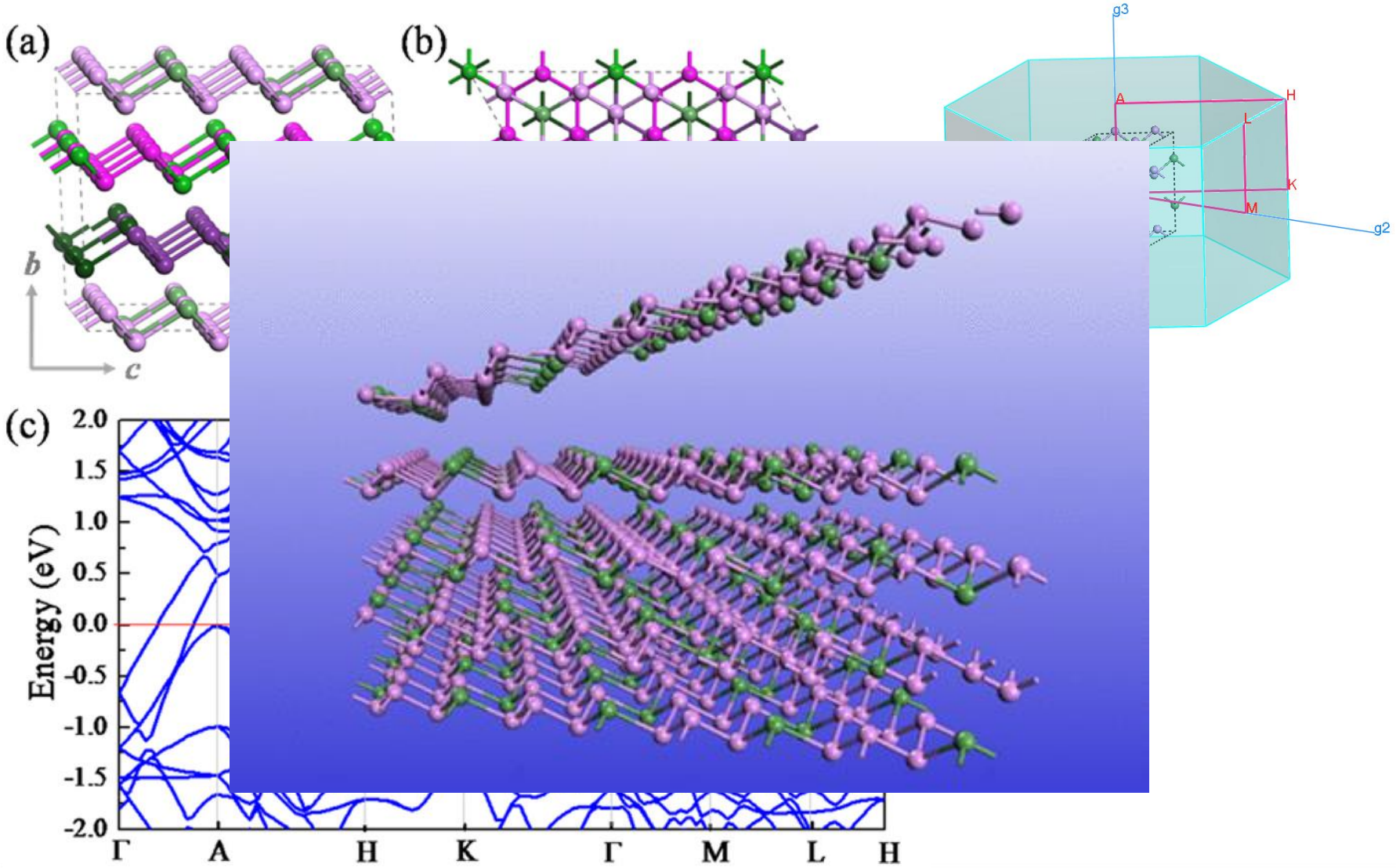


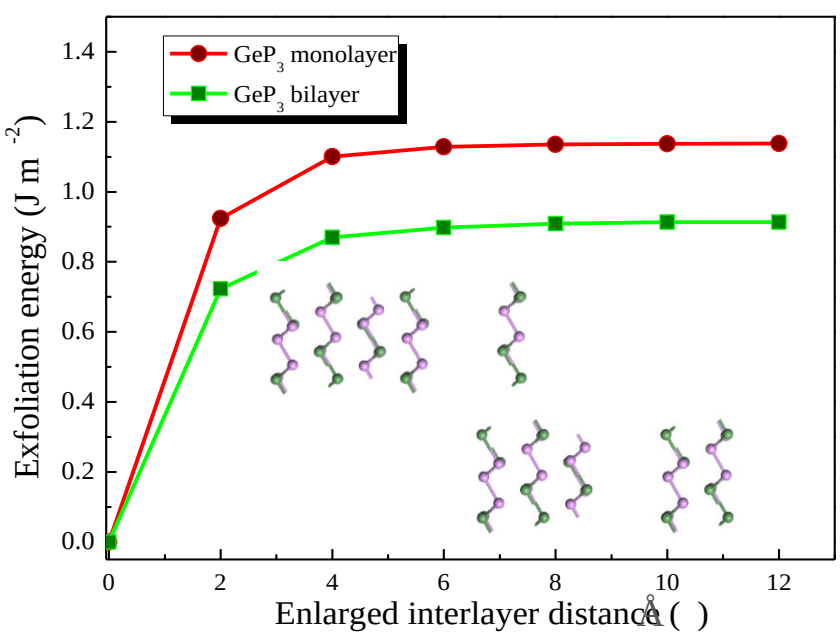
FIG. 1. The atomic arrangement in a puckered layer of SnP_3. Small circles represent phosphorus atoms and large circles represent tin atoms.

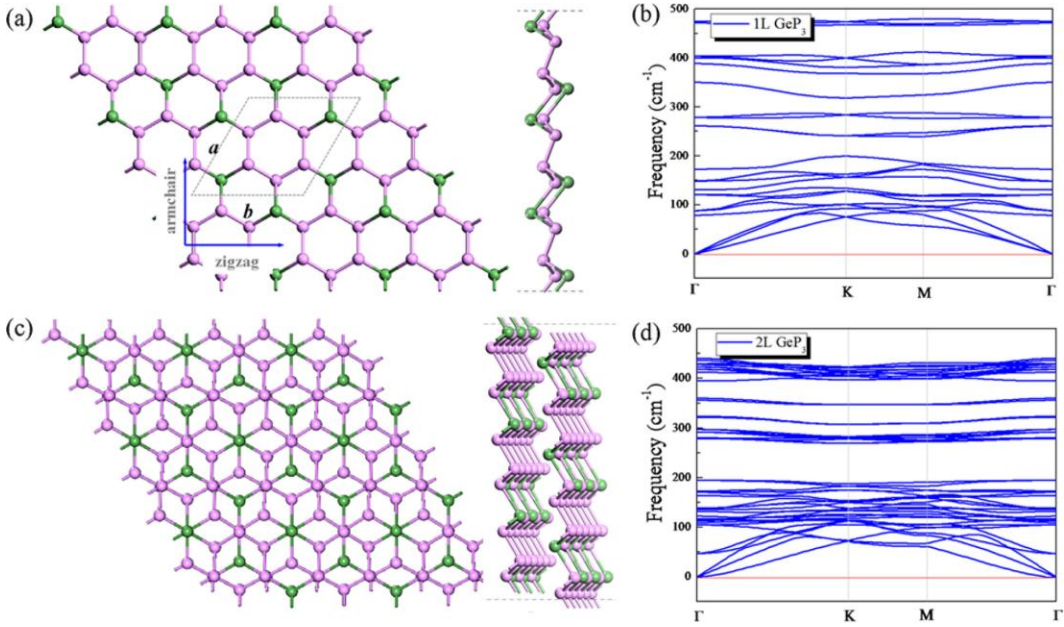
Bulk GeP_3



Yu Jing, Yandong Ma, Yafei Li, Thomas Heine, NanoLetters 17 (2017) 1833–1838

Exfoliation of GeP_3 (in silico)



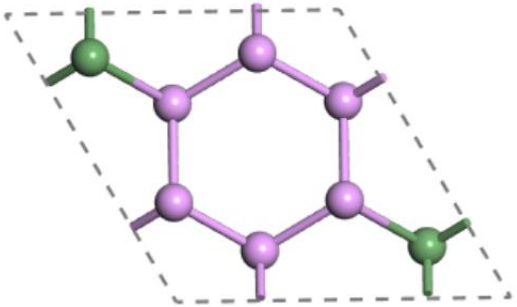


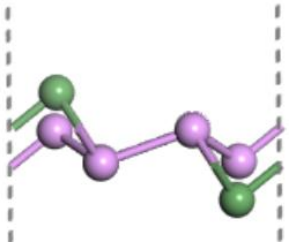
	GeP_3	GaN_2	NaSnP	Graphene
monolayer	1.14 J m^{-2}	1.09 J m^{-2}	0.81 J m^{-2}	0.37 J m^{-2}
bilayer	0.91 J m^{-2}			

Yu Jing, Yandong Ma, Yafei Li, Thomas Heine, NanoLetters 17 (2017) 1833–1838

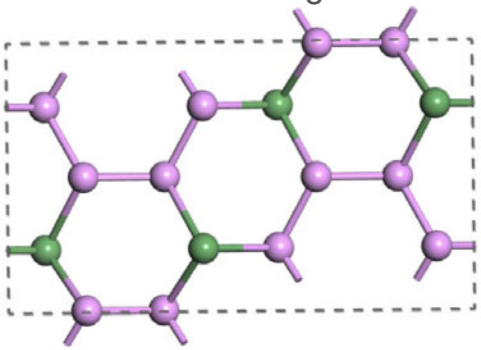
GeP_3

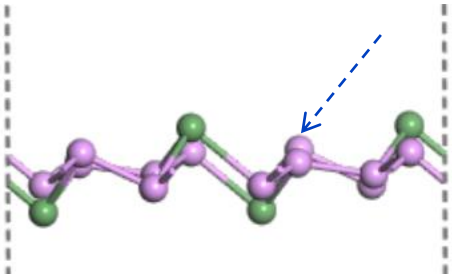
GeP_3 in a hexagonal cell



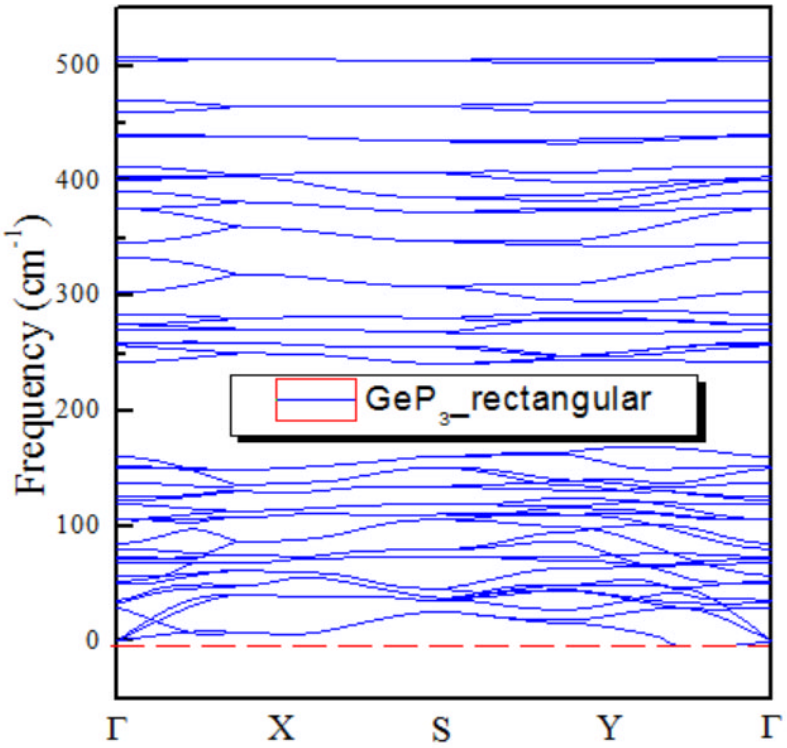


GeP_3 in a rectangular cell

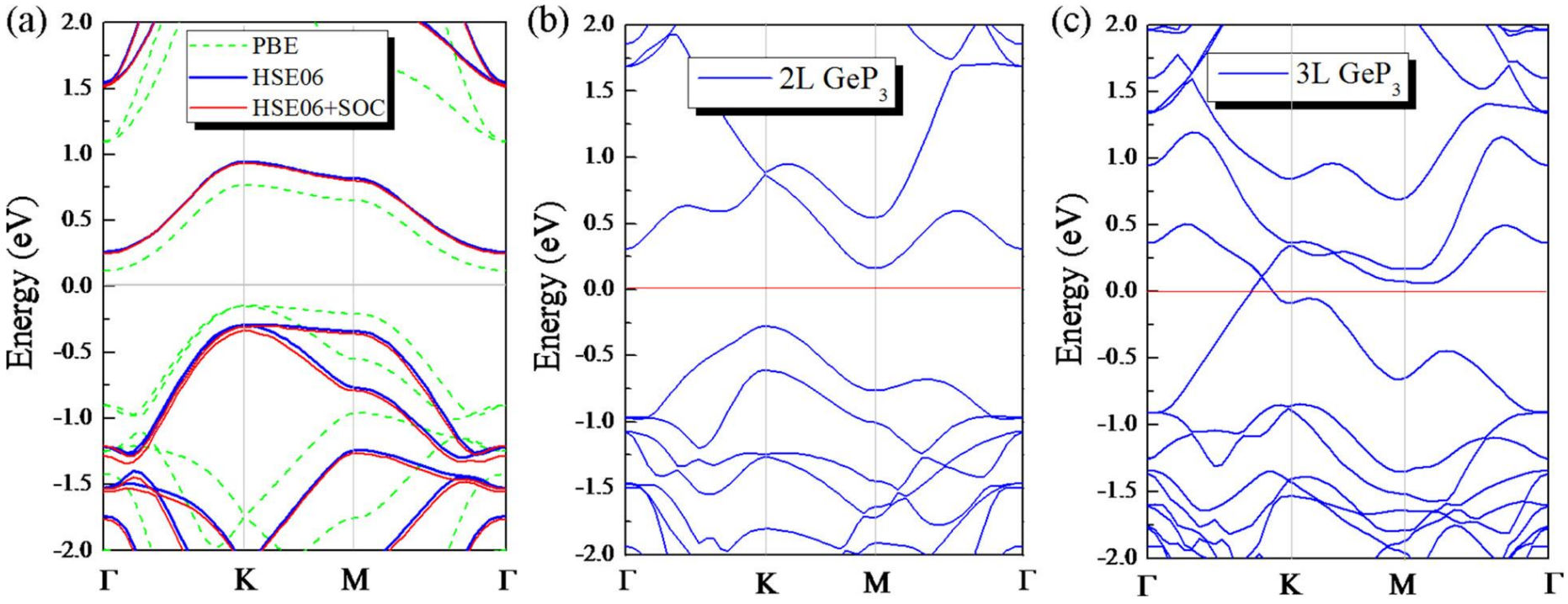




phonon spectrum (rect. cell)



Layer-dependent band structure



	Band gap ×eV	Electron mobility ×10³ cm²/(Vs)		Hole mobility ×10³ cm²/(Vs)	
		zig	arm	zig	arm
monolayer	~0.55	0.04	0.07	0.014 (0.35)	0.19 (0.36)
bilayer	~0.43	1.25	8.84	4.63	8.48

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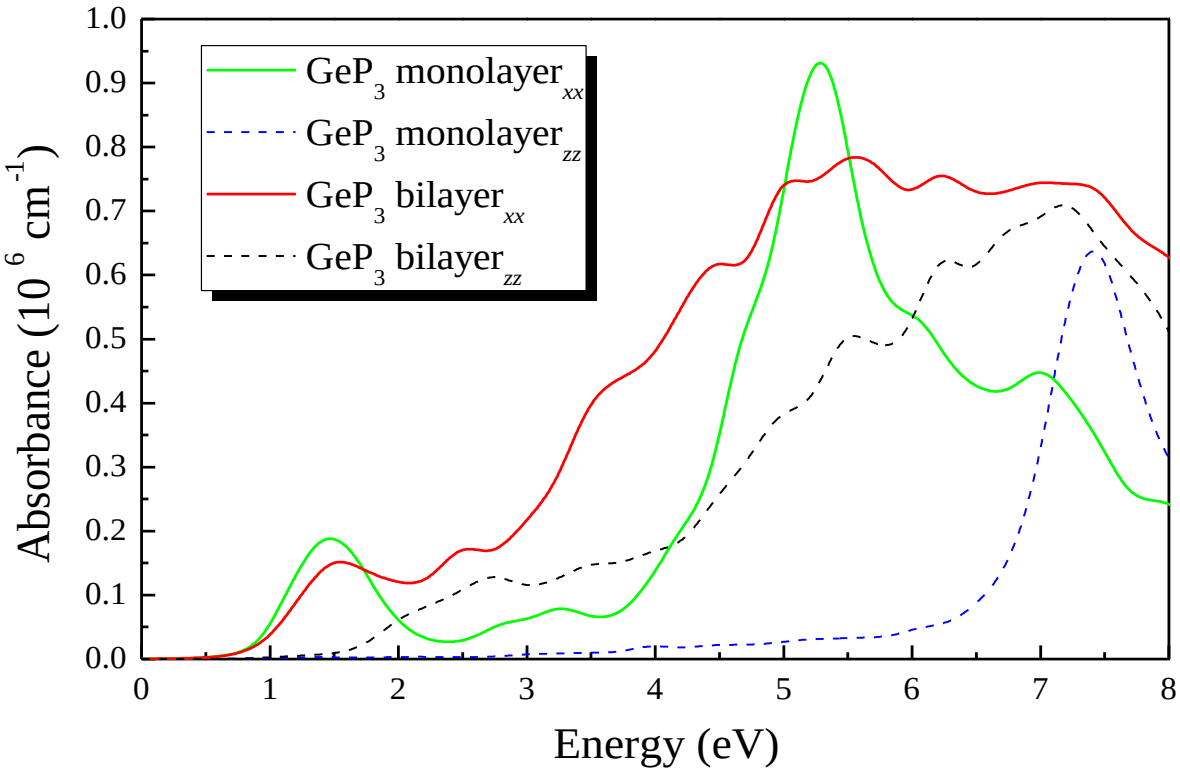
Light-harvesting capability



- GeP_3 thin layers are novel 2D materials that could be exfoliated from the bulk.
- They have band gaps in the range of 0.3~0.5 eV, which are layer-dependent and can be further tuned by biaxial elastic strain.
- They show high carrier mobiliies and pronounced light-harvesting abilities.

Yu Jing, Yandong Ma, Yafei Li, Thomas Heine, NanoLetters 17 (2017) 1833–1838


Dr. Mahdi Ghorbani-Asl, HZDR
Dr. Pere Miró, U South Dakota

Two Dimensional Materials Beyond MoS_2: Noble Transition Metal Dichalcogenides

P. Miró, M. Ghorbani-Asl, T. Heine

Angew. Chem. Intl. Ed. Engl. 53 (2014) 3015–3018

ACTA CHEMICA SCANDINAVICA 10 (1956) 1620—1634

On the Sulfides, Selenides and Tellurides of Palladium

FREDRIK GRØ

ACTA C

T
dium
X-ray
menta

High Ten

ACTA CHEMICA SCANDINAVICA 14 (1960) 1879—1893

On the Sulfides, Selenides and Tellurides of Platinum

FREDRIK GRØNVOLD, HAAKON HARALDSEN and ARNE KJEKSHUS

Kjemisk Institutt A, Universitetet i Oslo, Blindern, Norway

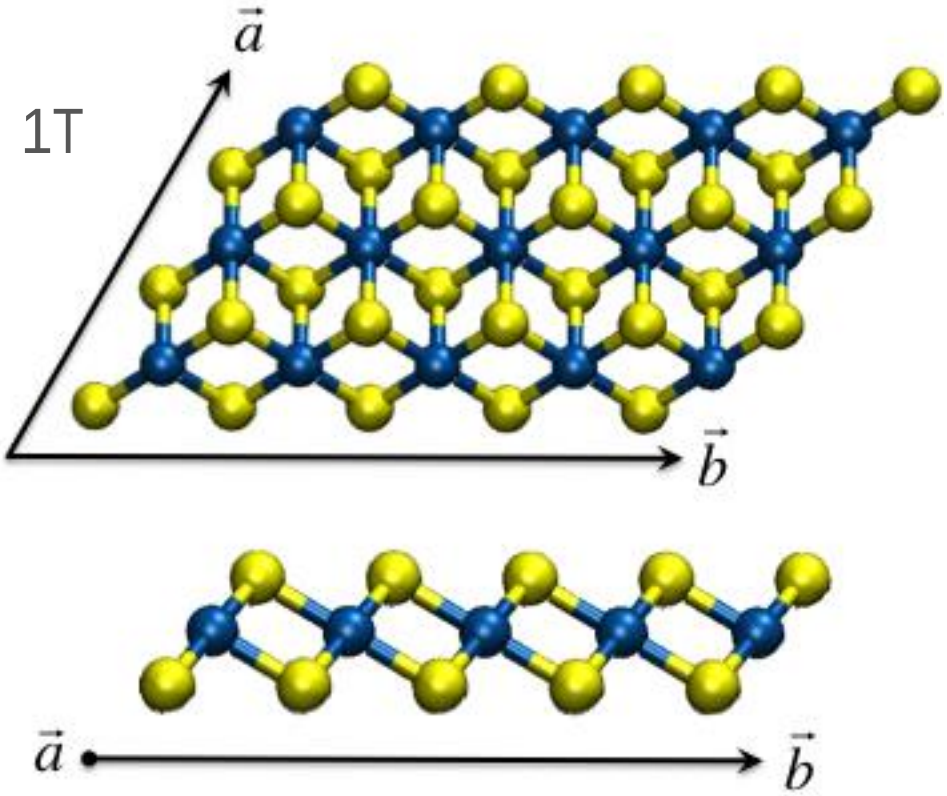
The phase relationships in the systems platinum sulfur, platinum selenium and platinum tellurium have been studied by means of X-rays. Density determinations and magnetic susceptibility measurements have been carried out. Two new, intermediate phases were identified:

1. $PtSe_{0.80}$, with monoclinic structure, $a = 6.5806$ Å, $b = 4.6248$ Å, $c = 11.145$ Å, $\beta = 78.40°$. The pycnometric density is 12.79 g cm^{-3} at 25°C. The unit cell contains ten formula units and the probable space group is Pc or $P2/c$.

2. PtTe, with orthorhombic structure, $a = 6.6144$ Å, $b = 5.6360$ Å, $c = 11.865$ Å. The observed density is 12.01 g cm^{-3}. The unit cell contains ten formula units.

The earlier known phases PtS, PtS_2, $PtSe_2$ and $PtTe_2$ have been reinvestigated. The lattice constants and the observed densities are:

Structure of Group 10 MX_2



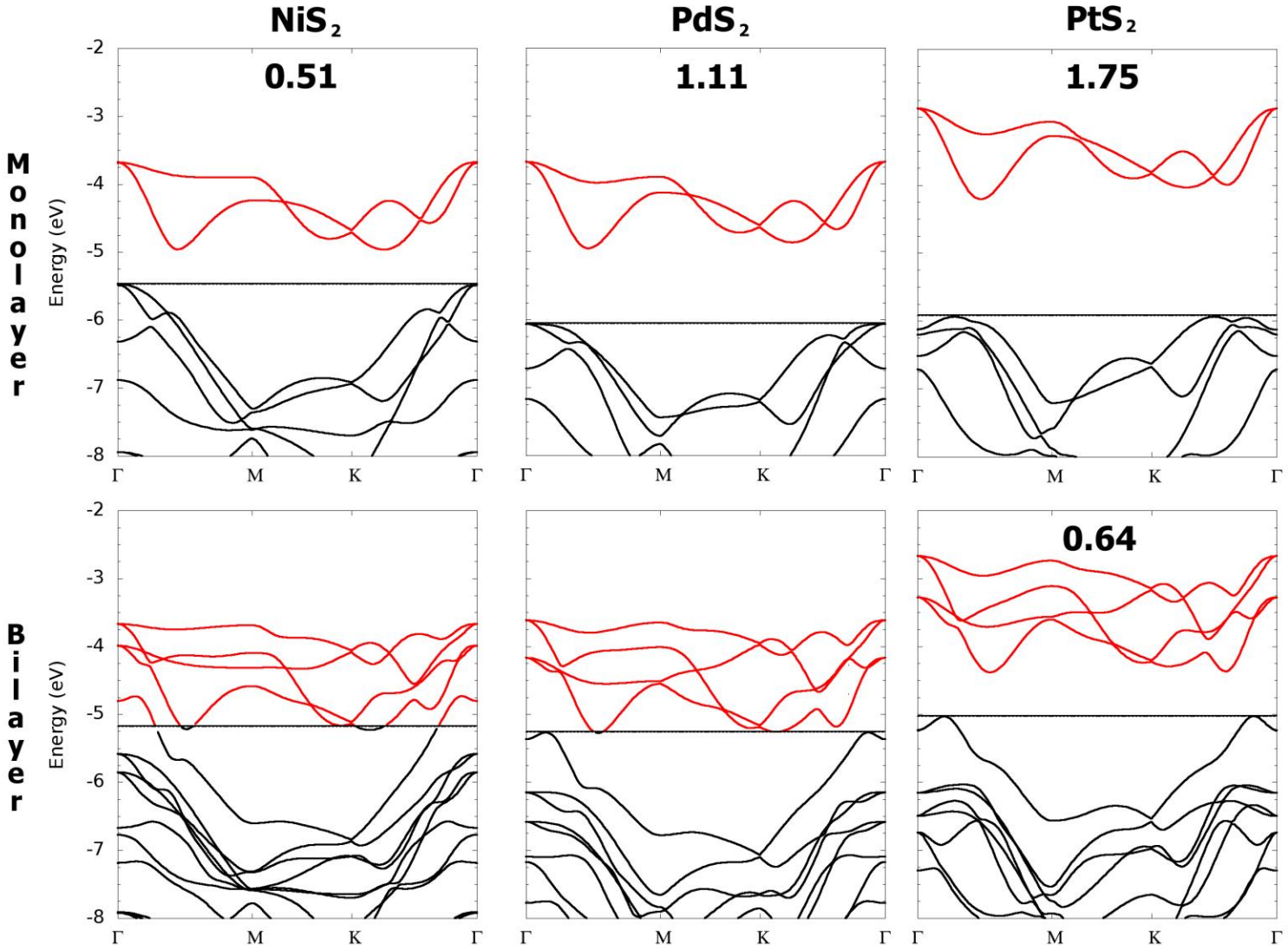
group 10

	28 Ni 58.7	
	46 Pd 106.4	
	78 Pt 195.1	

Groenvold and Kjekshus 1956-1960: PdX_2 and PtX_2, X=S, Se, have a layered structure. Ni does not (we include it for completeness)

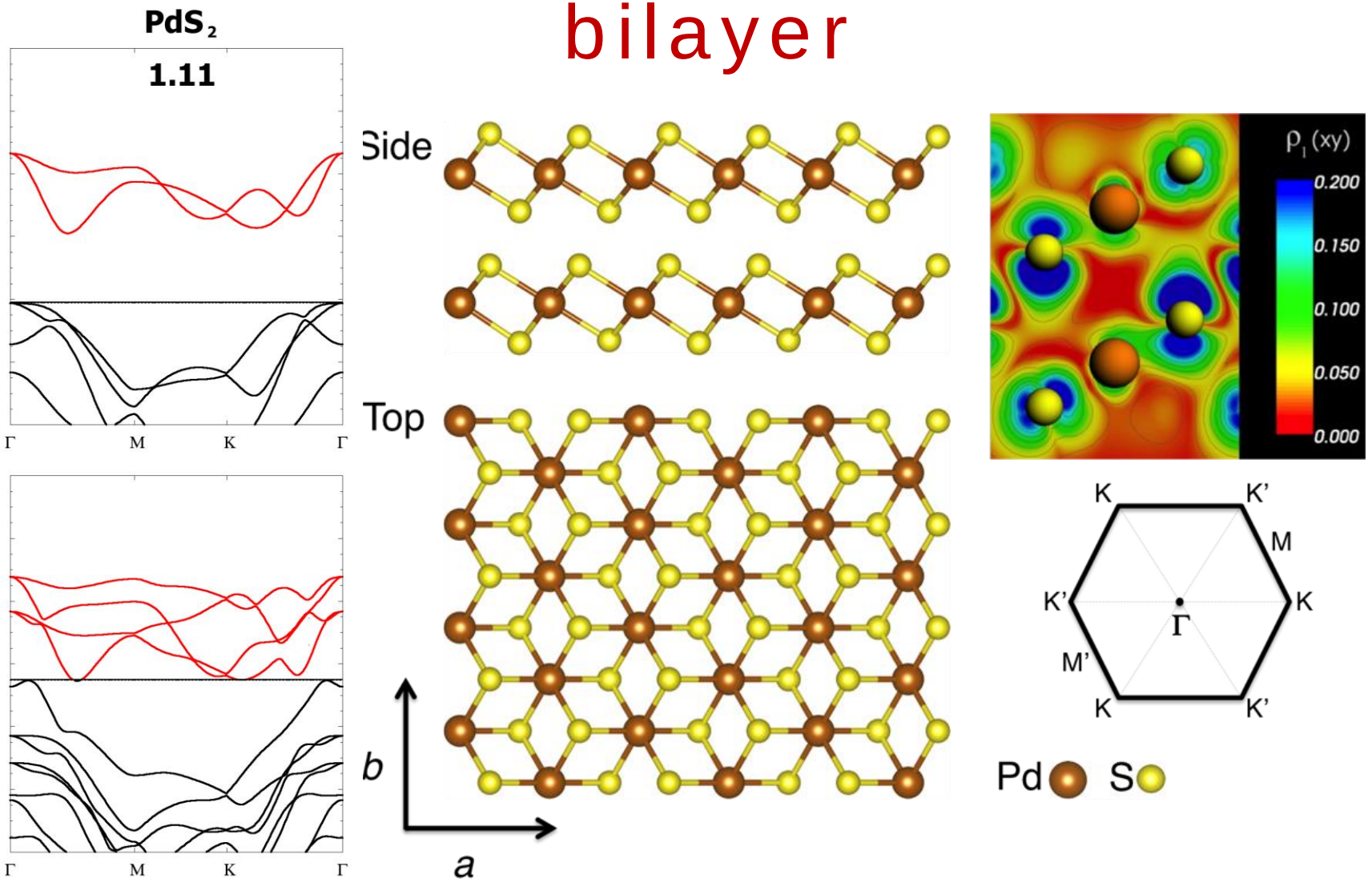
F. Groenvold, E. Rost, Acta Chem. Scand. 1956, 10, 1620;
A. Kjekshus, F. Groenvold, Acta Chem. Scand. 1959, 13, 1767;
F. Groenvold, H. Haraldsen, A. Kjekshus, Acta Chem. Scand. 1960, 14, 1879.

Band Structure of Group 10 MX_2



P. Miró, M. Ghorbani-Asl, T. Heine, Angew. Chem. Intl. Ed. 53 (2014) 3015–3018

Interlayer interactions in PdS_2 bilayer



P. Miró, M. Ghorbani-Asl, T. Heine, Angew. Chem. Intl. Ed. 53 (2014) 3015–3018

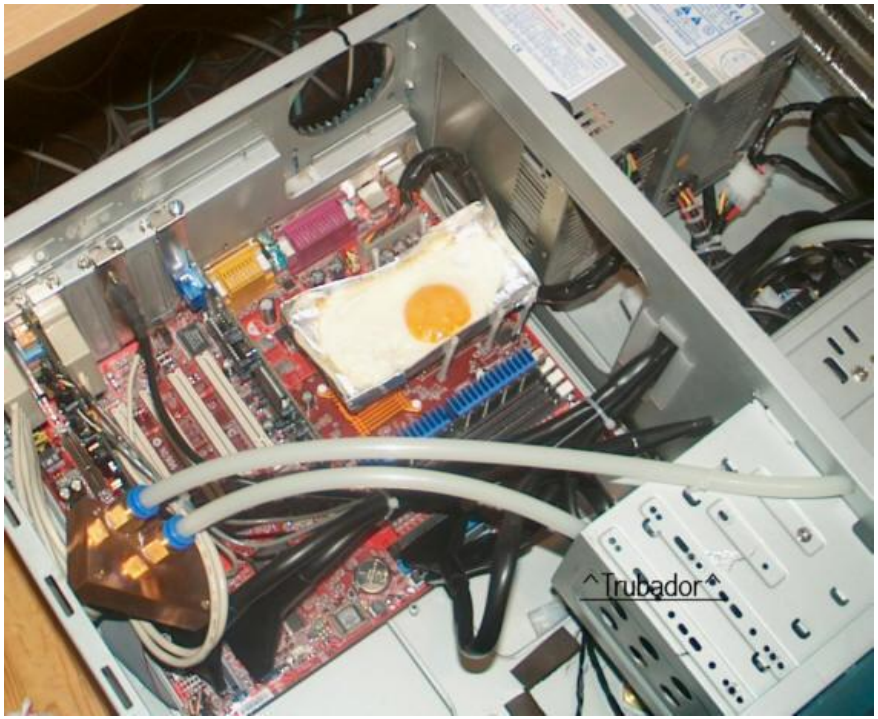
Advances of cooling technology

today

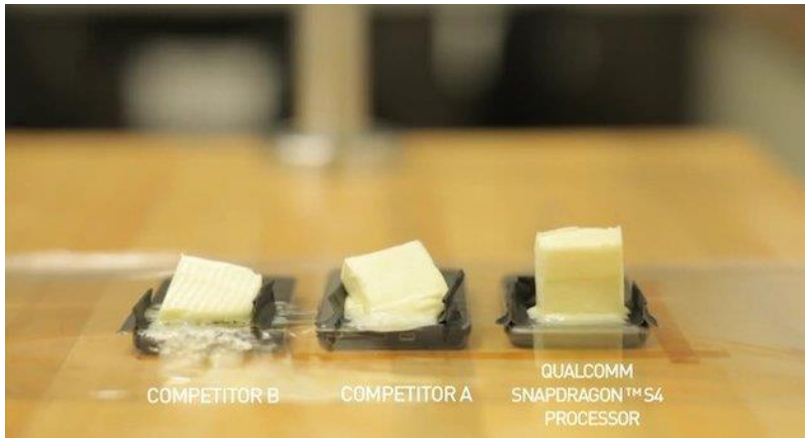
1993

Heat dissipation is another challenge for high integration

Heat dissipation due to leak currents and contact resistance

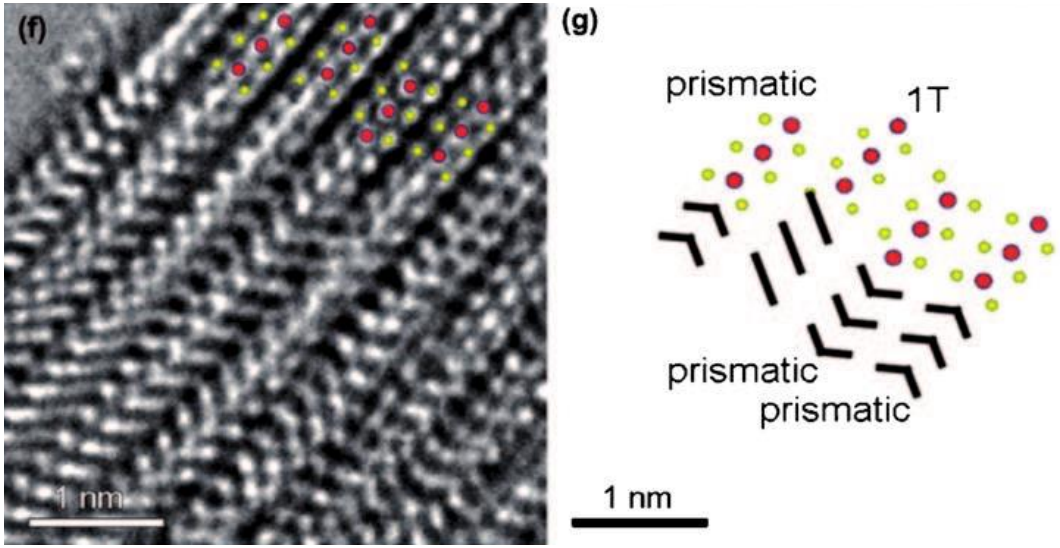


Source: http://www.phys.ncku.edu.tw/



Source: QUALCOMM

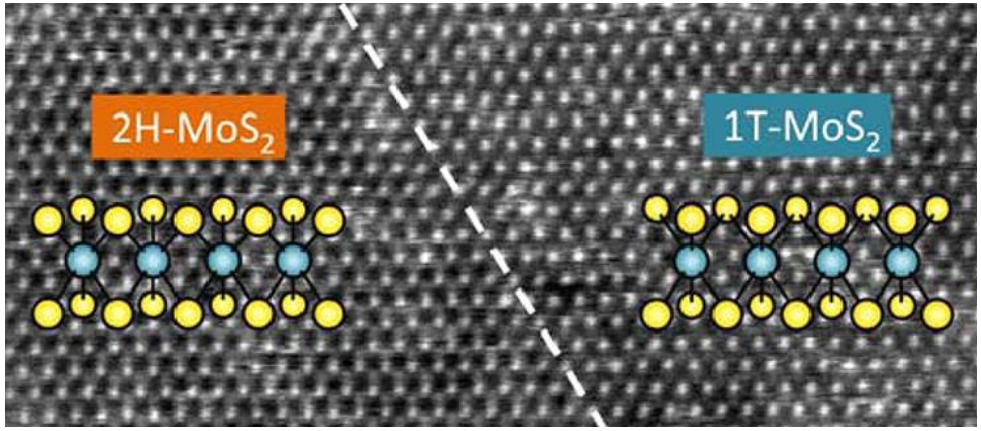
Design idea by Andras Kis, EPFL



Albu-Yaron et al. Angew. Chem. Int. Ed. 50, 1810 (2011)

"HRTEM showing atomic resolution of the MoS_2 layers. The atomic model is overlaid in red (Mo) and yellow (S), and detailed in (g) with black lines as visual guides to their appearance in the TEM image. The chevron motif correlates with a prismatic coordinated MoS_2 layer, which as a bulk phase is semiconducting. The pattern of diagonal lines indicates the 1T phase, which has been predicted to be metallic."

"High resolution scanning transmission electron microscope (STEM) imaging reveals the coexistence of metallic and semiconducting phases within the chemically homogeneous two-dimensional (2D) MoS_2 nanosheets."



Eda et al. ACS Nano 6, 7311 (2012)

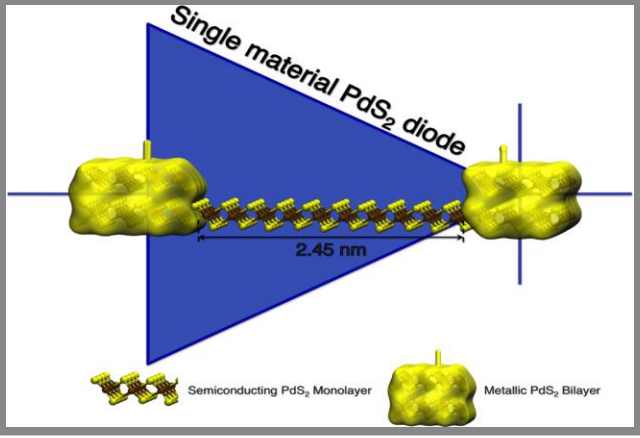


Dr. Mahdi Ghorbani-Asl, Dr. Agnieszka Kuc, Dr. Pere Miró

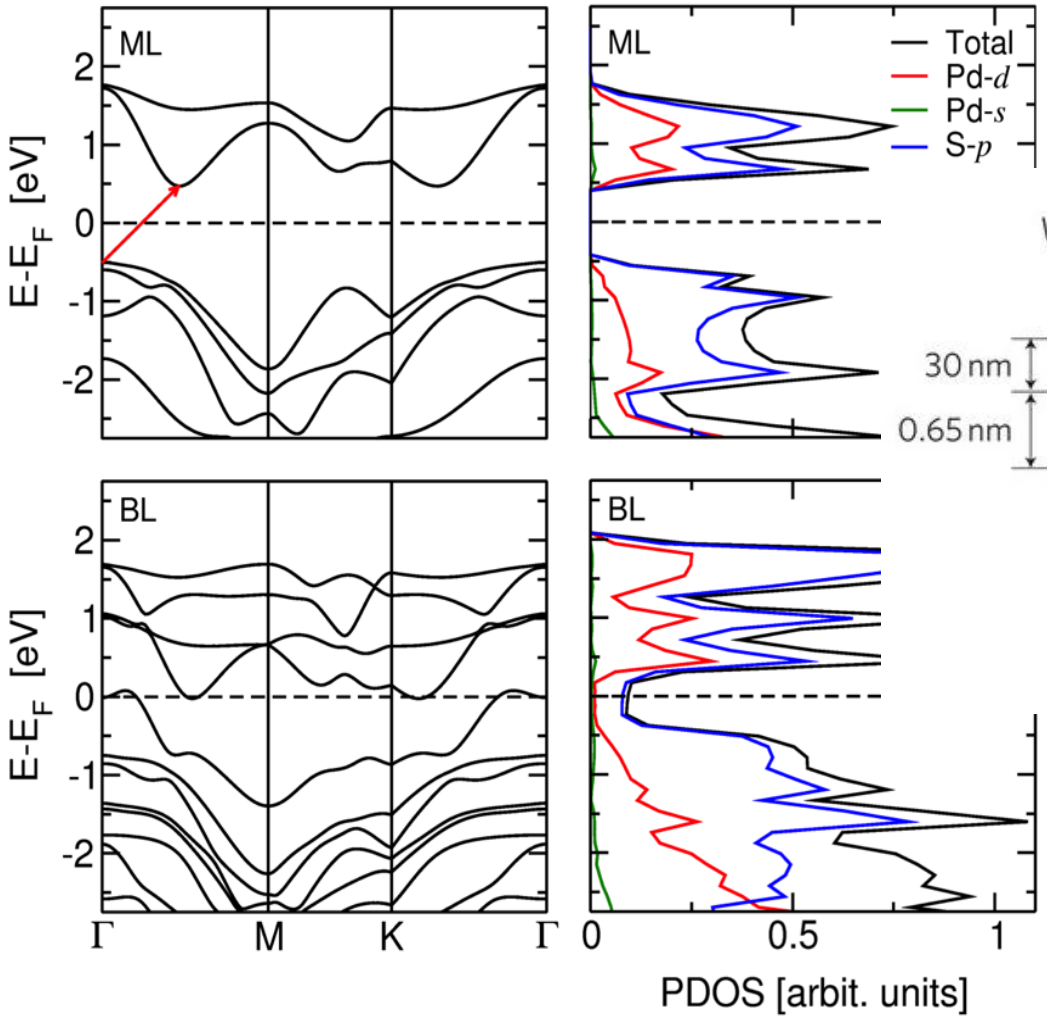
U Cambridge Northwestern U

Use quantum confinement for low-energy logical junctions

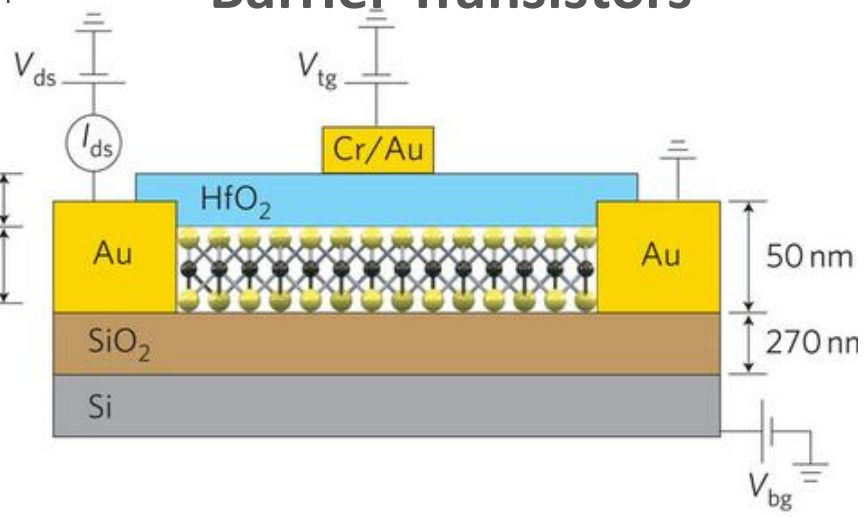
Adv. Materials 28 (2016) 853–856.



Electronic properties of PdS_2



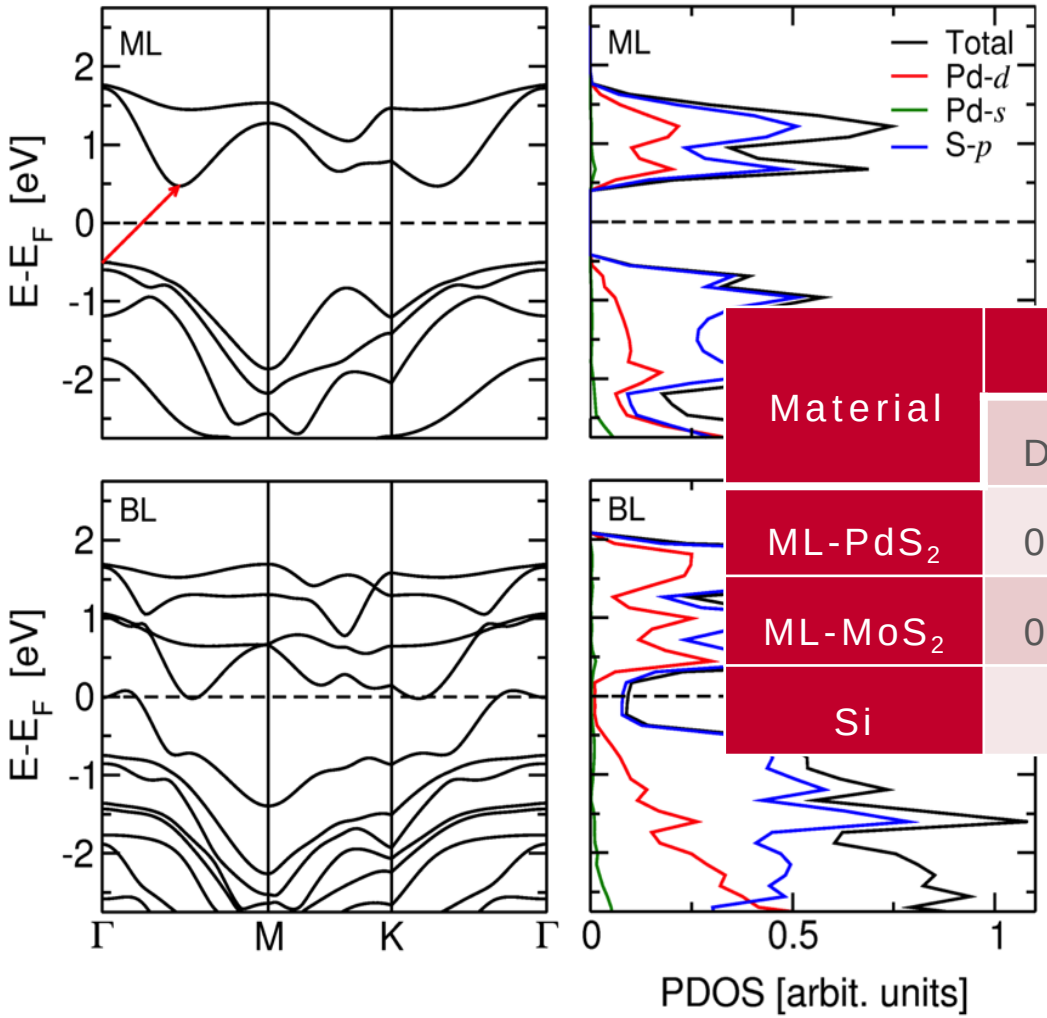
Idea: quasi-zero Schottky Barrier Transistors



Schottky barrier is a potential energy barrier for electrons formed at a metal–semiconductor junction.

M. Ghorbani-Asl, A. Kuc, P. Miró, T. Heine, Adv. Materials 28 (2016) 853–856.

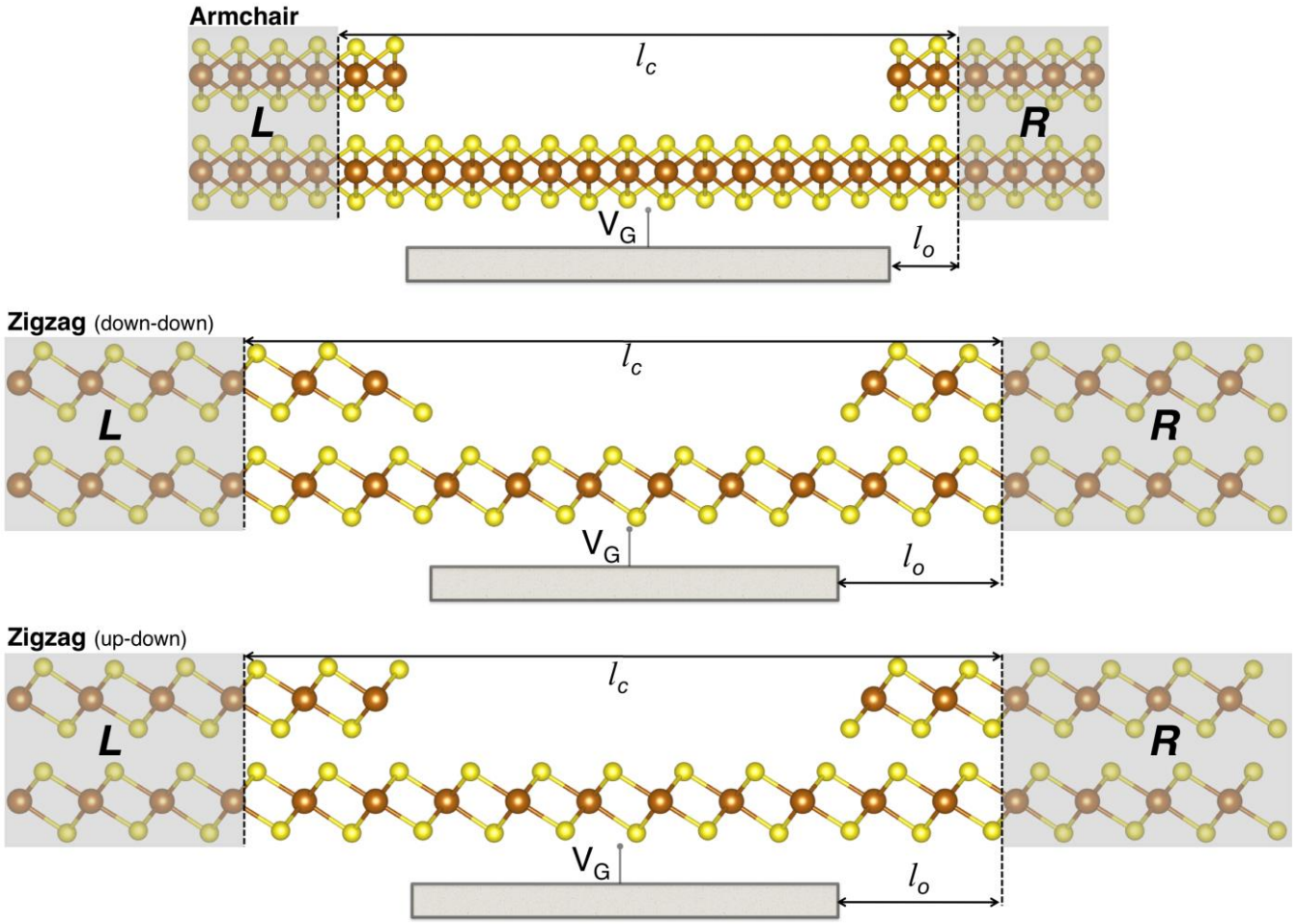
Electronic properties of PdS_2



Material	m_e^*/m_0		m_h^*/m_0	
	Down	Up	Down	Up
ML-PdS_2	0.467	0.467	-1.342	-1.342
ML-MoS_2	0.460	0.525	-0.621	-0.542
Si	0.26		-0.36	

M. Ghorbani-Asl, A. Kuc, P. Miró, T. Heine, Adv. Materials 28 (2016) 853–856.

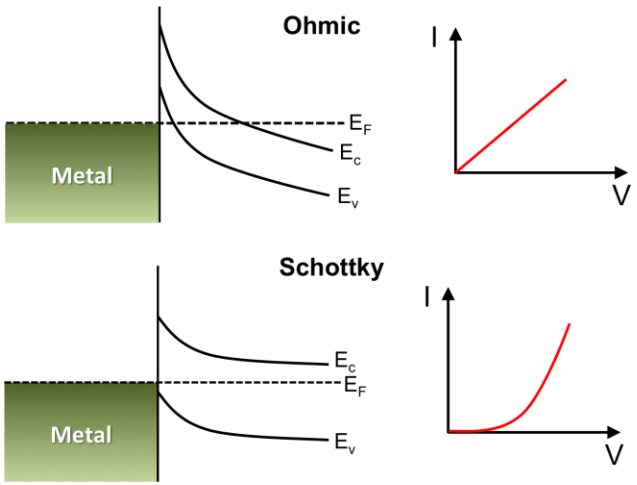
Model Systems – NEGF Transport

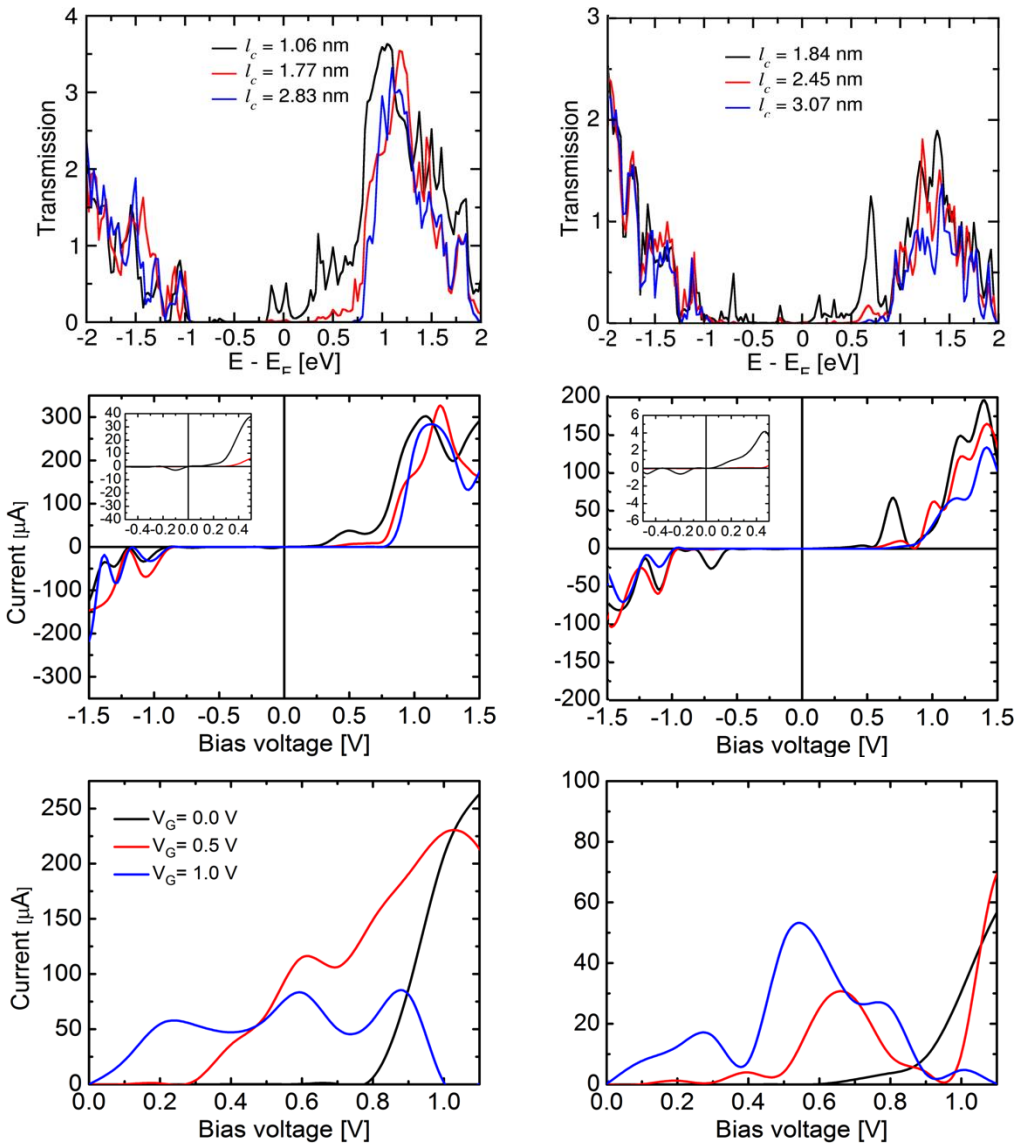


Electronic Transport

- Other studied models show similar behavior

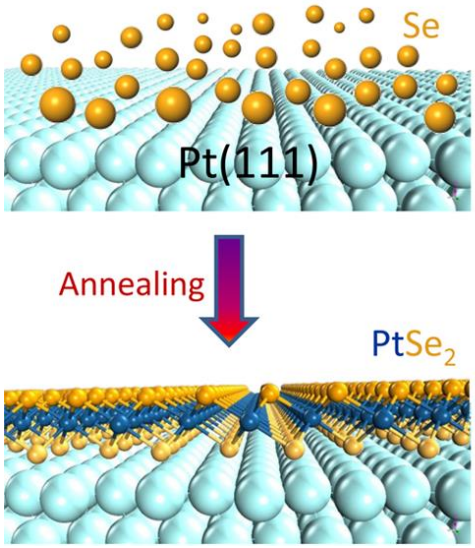
- Gate voltage changes the I-V characteristics to Ohmic





M. Ghorbani-Asl, A. Kuc, P. Miró, T. Heine, Adv. Materials 28 (2016) 853–856.

Synthesis of $PtSe_2$ by self-terminating Se deposition

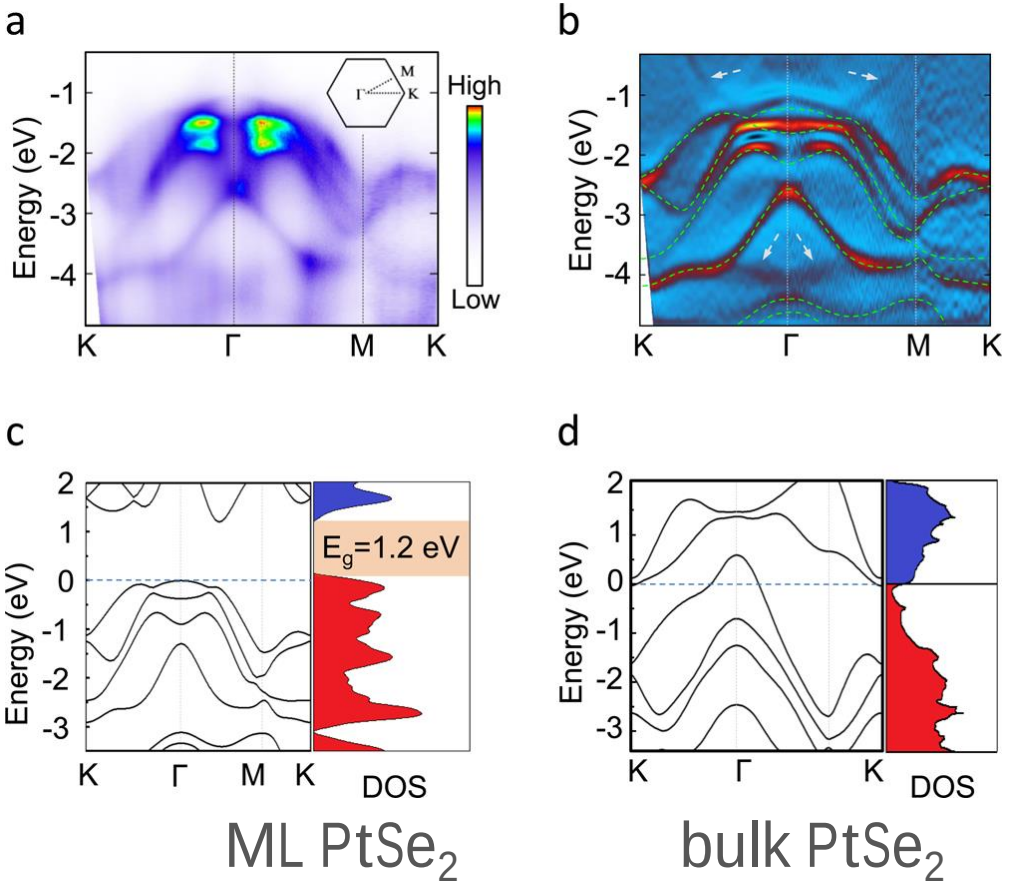


"In summary, we have successfully fabricated high-quality, single-crystalline, monolayer $PtSe_2$ films,

a new member of the TMDs family,

through a single-step, direct selenization of a Pt(111) substrate at a relatively low temperature (~270 ° C)."

ML $PtSe_2$ on Pt(111)



Wang et al. Nano Lett. 15, 4013 (20125)

Synthesis of PtS_2

Materials Views
www.MaterialsViews.com

ADVANCED MATERIALS
www.advmat.de

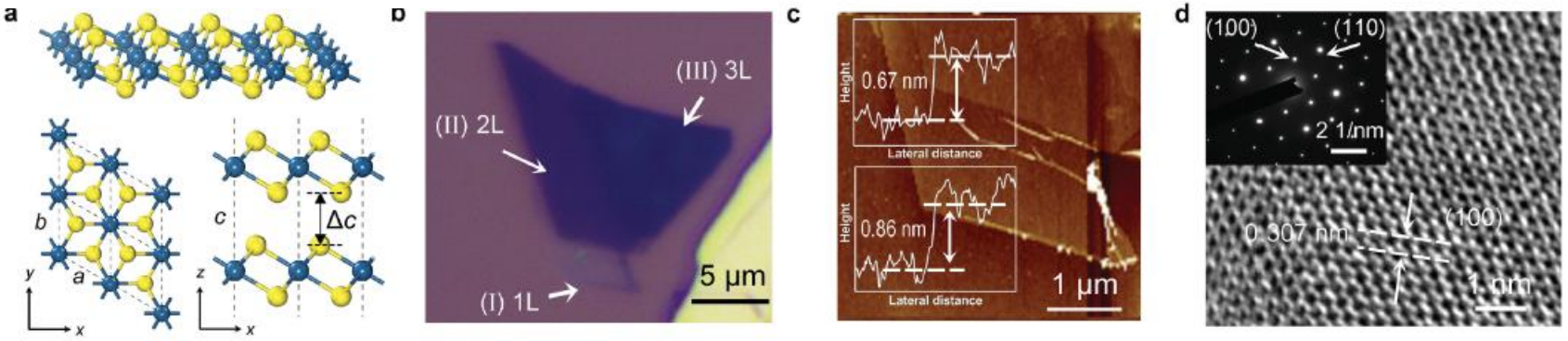
COMMUNICATION

Extraordinarily Strong Interlayer Interaction in 2D Layered PtS_2

Yuda Zhao, Jingsi Qiao, Peng Yu, Zhixin Hu, Ziyuan Lin, Shu Ping Lau, Zheng Liu, Wei Ji, and Yang Chai**

The interlayer interaction in 2D layered materials (2DLMs) can dramatically affect the intralayer bonding, band-structures, and lattice vibrations of the 2DLMs, exhibiting distinct layer-

high as 1107 $cm^2 V^{-1} s^{-1}$ at room temperature,[20–22] a fundamental understanding on the layer-dependent properties of group-10 TMDs and the effect of *d*-electron count on the inter-



Band gap:

Monolayer – Indirect - ~1.6 eV

Bulk – Indirect - ~0.2 eV

Literature follow-up

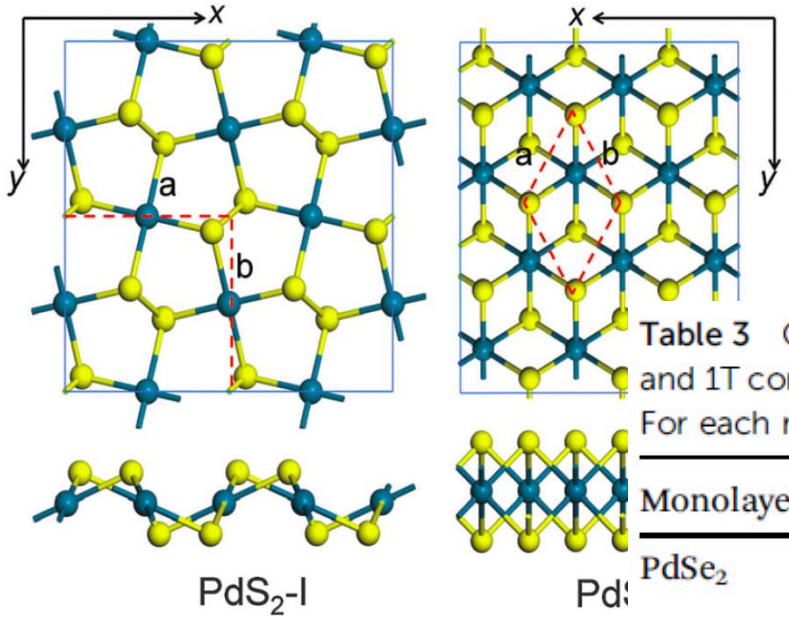


Fig. 1 Top (upper) and side (bottom) views of the tw
PdS_2 monolayer. Black green and yellow balls represe
respectively. Both monolayers are extended periodical
directions.

Table 1 The optimized lattice parameters (LP), length
S–S (d_{S-S}) bonds, and relative energy (E_r) of two co
PdS_2 monolayer

Polytype	LP (Å)	d_{Pd-S} (Å)	d_{S-S} (Å)
PdS_2-I	$a = 5.49$, $b = 5.59$	2.34, 2.35	2.10
PdS_2-II	$a = b = 3.53$	2.40	—

Table 3 Optimized lattice parameters and relative energies for PdS_2-type and 1T configurations of $PdSe_2$, $PdTe_2$, PtS_2, $PtSe_2$, and $PtTe_2$ monolayers. For each monolayer, the enengy of 1T configuration was set as zero

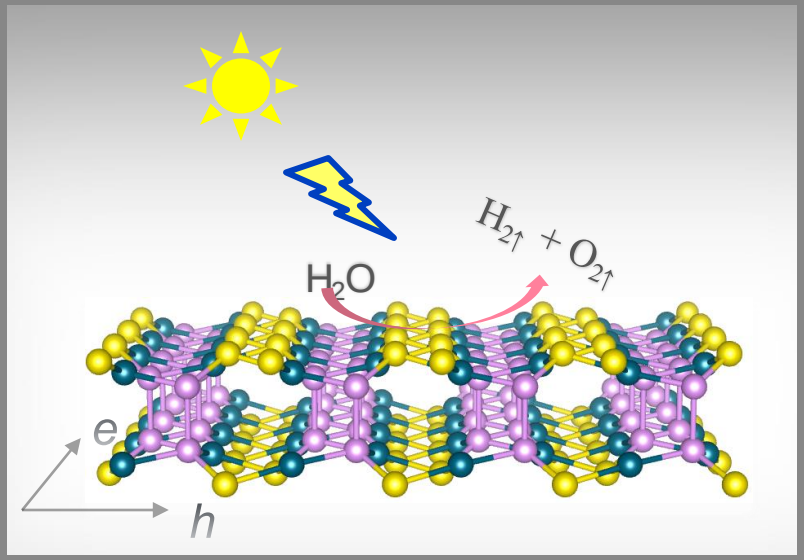
Monolayer	Configuration	LP (Å)	E_r (meV per atom)
$PdSe_2$	PtS_2-type	$a = 5.74$, $b = 5.92$	−25
	1T	$a = b = 3.74$	0
$PdTe_2$	PtS_2-type	$a = 5.99$, $b = 6.37$	15
	1T	$a = b = 4.03$	0
PtS_2	PtS_2-type	$a = 5.47$, $b = 5.56$	45
	1T	$a = b = 3.58$	0
$PtSe_2$	PtS_2-type	$a = 5.73$, $b = 5.91$	102
	1T	$a = b = 3.75$	0
$PtTe_2$	PtS_2-type	$a = 5.97$, $b = 6.35$	113
	1T	$a = b = 4.02$	0

Y. Wang, Y. Li, Z. Chen, J. Mater. Chem. C 3 (2015) 9603.

Two Dimensional PdPX for Water Splitting

Yu Jing, Yafei Li, Thomas Heine

Submitted (2017).



JOURNAL OF SOLID STATE CHEMISTRY 3, 300–307 (1971)

Palladium and Platinum Phosphochalcogenides—Synthesis and Properties*

T. A.

Centra
Experi

JOURNAL OF SOLID STATE CHEMISTRY 68, 28–37 (1987)

A

Photoelectrochemical Characterization of Several Semiconducting Compounds of Palladium with Sulfur and/or Phosphorus

J. C. W. FOLMER,* J. A. TURNER, AND B. A. PARKINSON†

Photoconversion Research Branch, Solar Energy Research Institute, 1617 Cole Boulevard, Golden, Colorado 80401

Received February 13, 1985; in revised form June 18, 1986

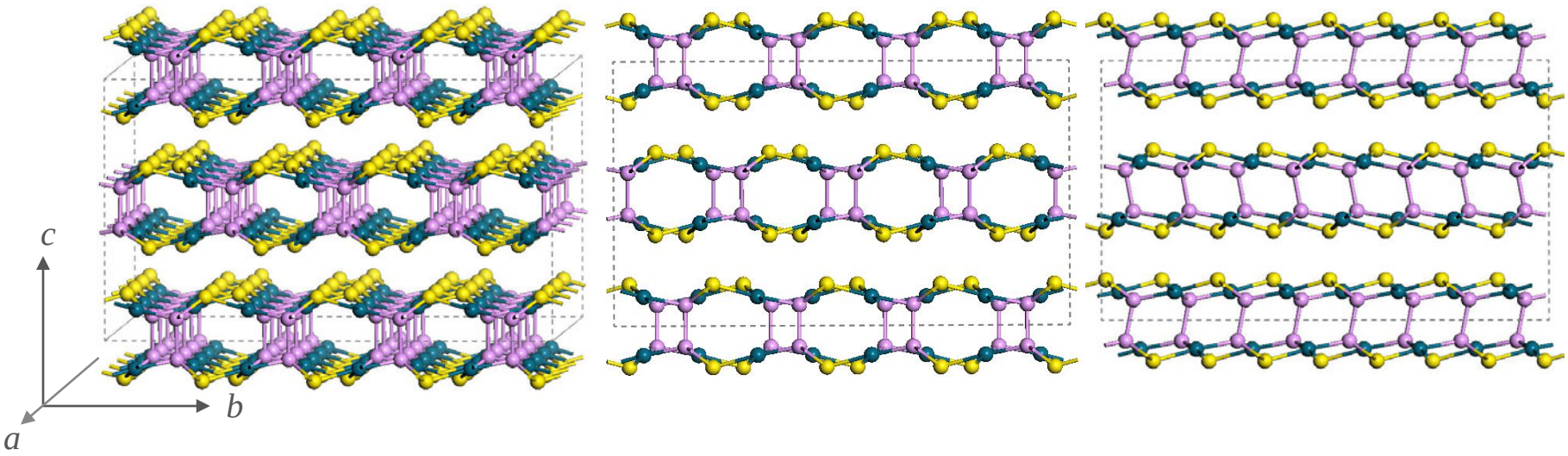
IT, AND

Semiconducting compounds of palladium with sulfur and/or phosphorus were prepared as crystals and their semiconducting and photoelectrochemical properties studied. The compounds include PdS, PdPS, $Pd_3(PS_4)_2$, and PdP_2 and crystal growth was accomplished by chemical vapor transport with halogens and Bridgeman methods. Photoelectrochemical techniques were used to measure bandgap, transition type, doping level, majority carrier type, flatband potential, quantum yield for electron flow, and stability in a photoelectrochemical cell. The previously undetermined bandgap of PdP_2 is reported (1.08 eV, indirect).

rammelsbergite and PdP
of the lone pair of S of o
bining the bonding chara

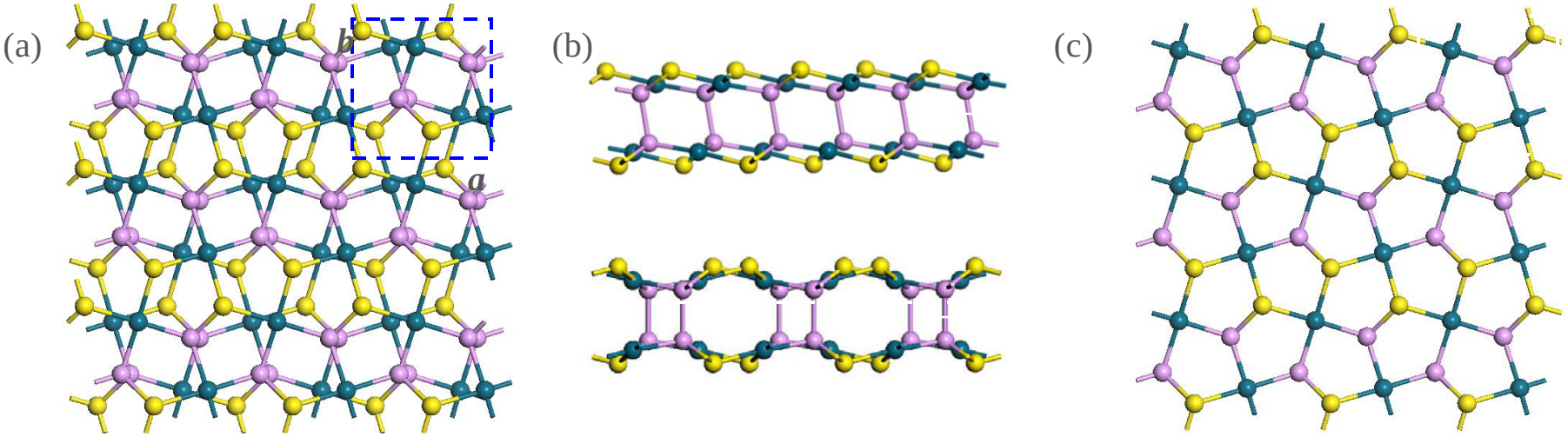
Single crystals of PdPSe were shown to be *n*-type semiconductors. Weak Pauli paramagnetic behavior was observed, which is consistent with the presence of delocalized electrons. Electrical measurements showed a room-temperature resistivity $\rho = 70$ ohm-cm, activation energy of resistivity $E_a = 0.32$ eV, and Hall mobility $\mu = 34\ cm^2\ V^{-1}\ sec^{-1}$. Photoelectronic measurements in aqueous solutions of I^-/I_3^- indicate that PdPSe has high quantum efficiencies below 800 nm. The indirect optical band gap is 1.28(2) eV.

Bulk PdPX, X = S, Se



Bulk PdPX are semiconductors with band gap of 1.70 and 1.43 eV for PdPS and PdPSe, respectively.

PdPX (X = S, Se) monolayer



Note: surface is similar to that of PdS_2(I) suggested by Chen et al.

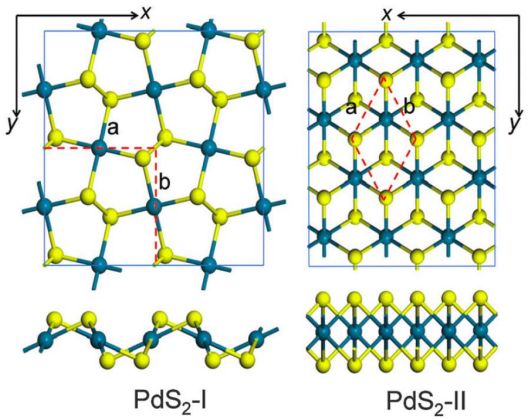
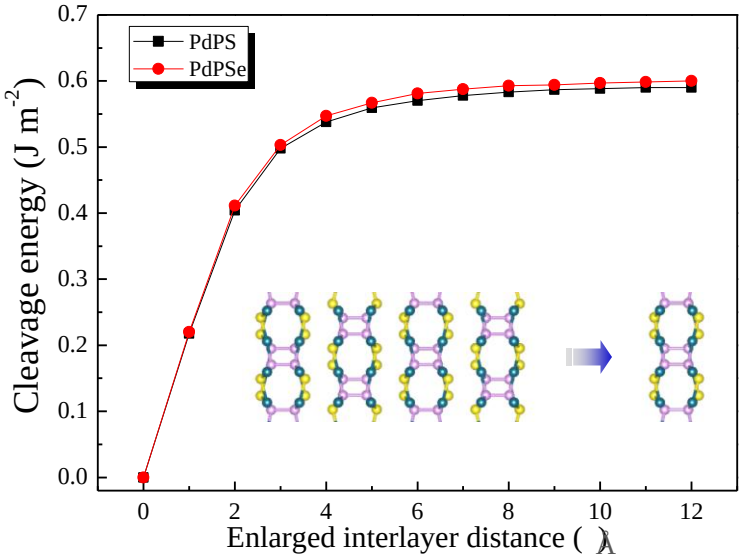
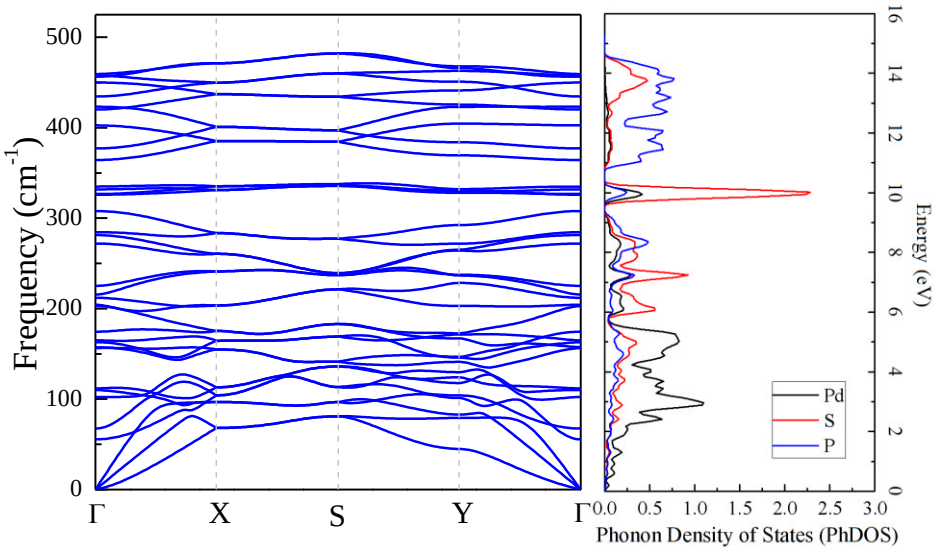


Fig. 1 Top (upper) and side (bottom) views of the two structures of the PdS_2 monolayer. Black green and yellow balls represent Pd and S atoms, respectively. Both monolayers are extended periodically along the *x* and *y* directions.

← Y. Wang, Y. Li, Z. Chen, J. Mater. Chem. C 3 (2015) 9603.

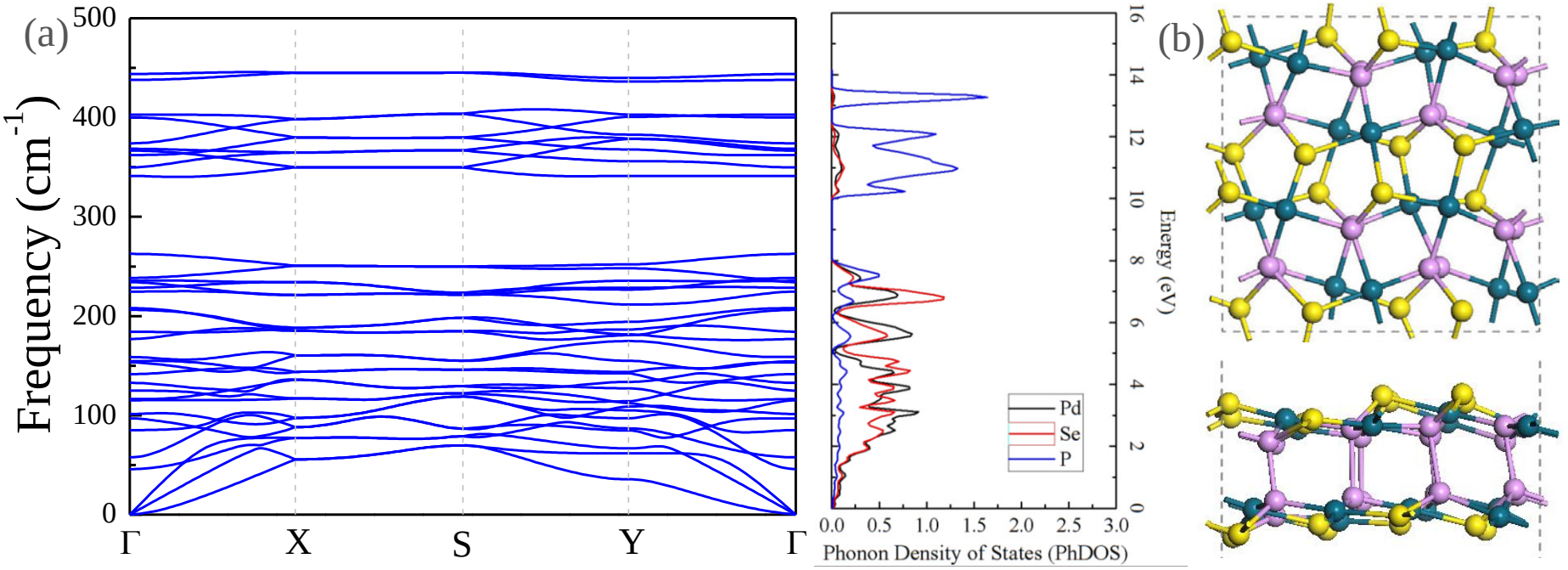
Cleavage energy and stabily



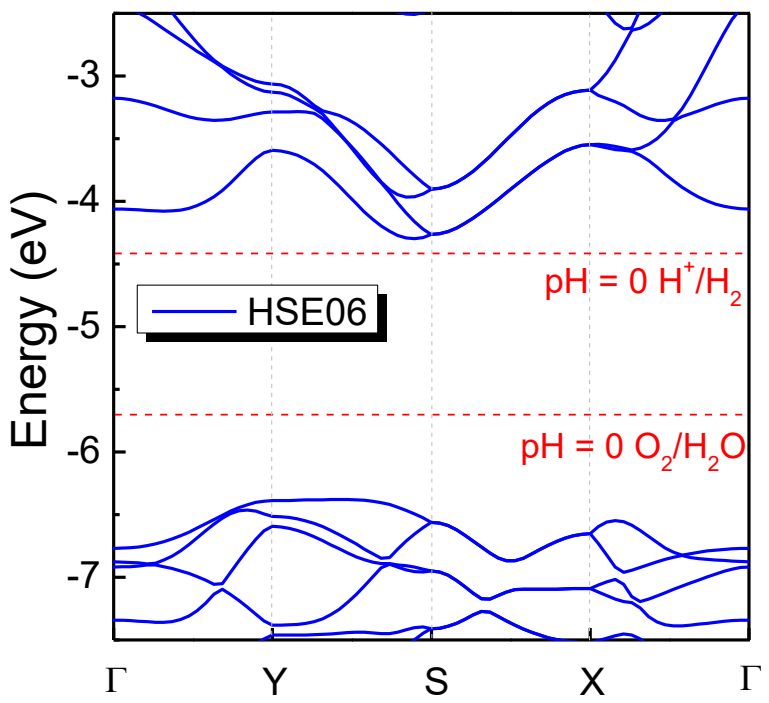


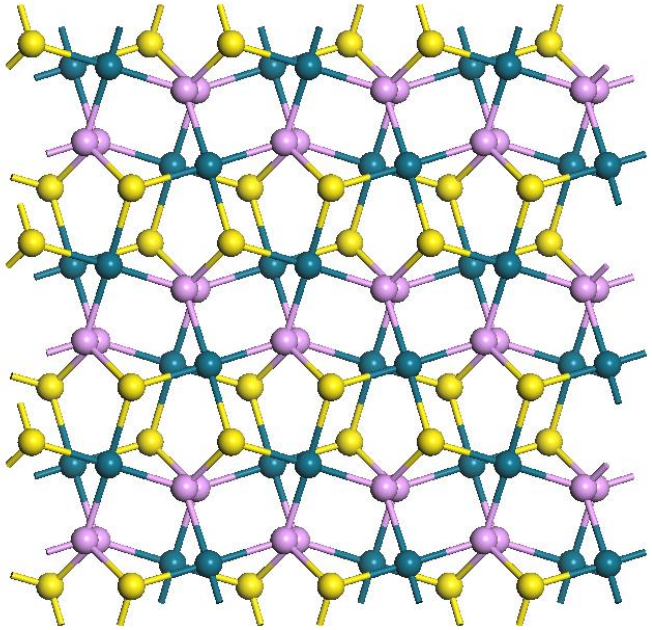
cleavage energy	PdPX ML	graphene	Ga_2N	NaSnP
J m^{-2}	~0.60	0.37	1.09	0.81

Stability


(a)
Frequency (cm-1)
500
400
300
200
100
0
Γ
X
S
Y
Γ
Pd
Se
P
0.0
0.5
1.0
1.5
2.0
2.5
3.0
Phonon Density of States (PhDOS)
Energy (eV)
16
14
12
10
8
6
4
2
0
(b)

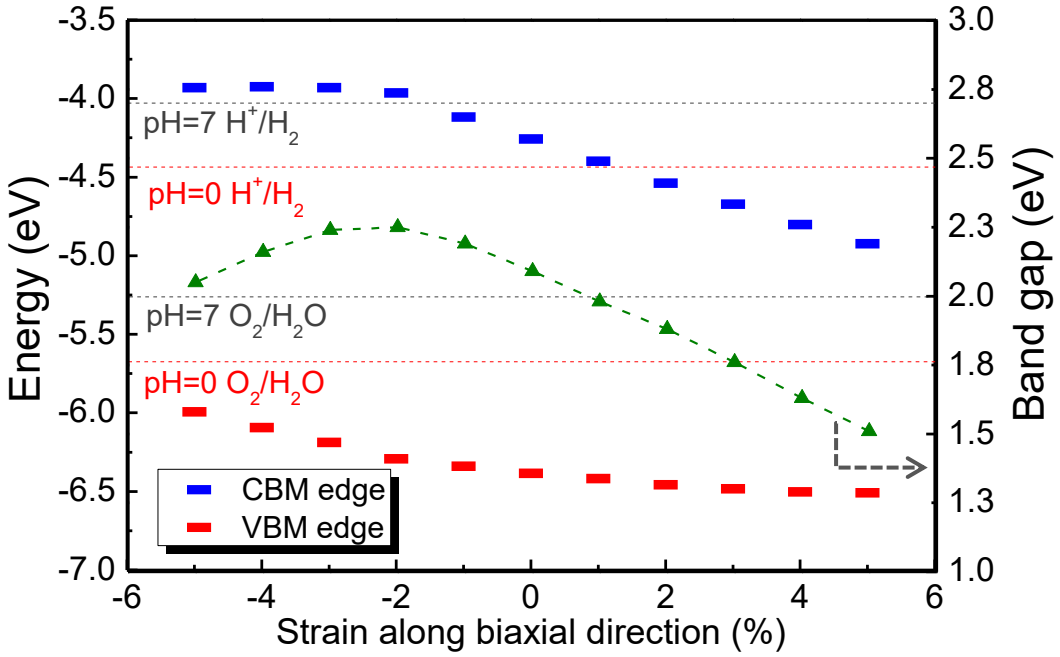
Band structure of PdPS monolayer





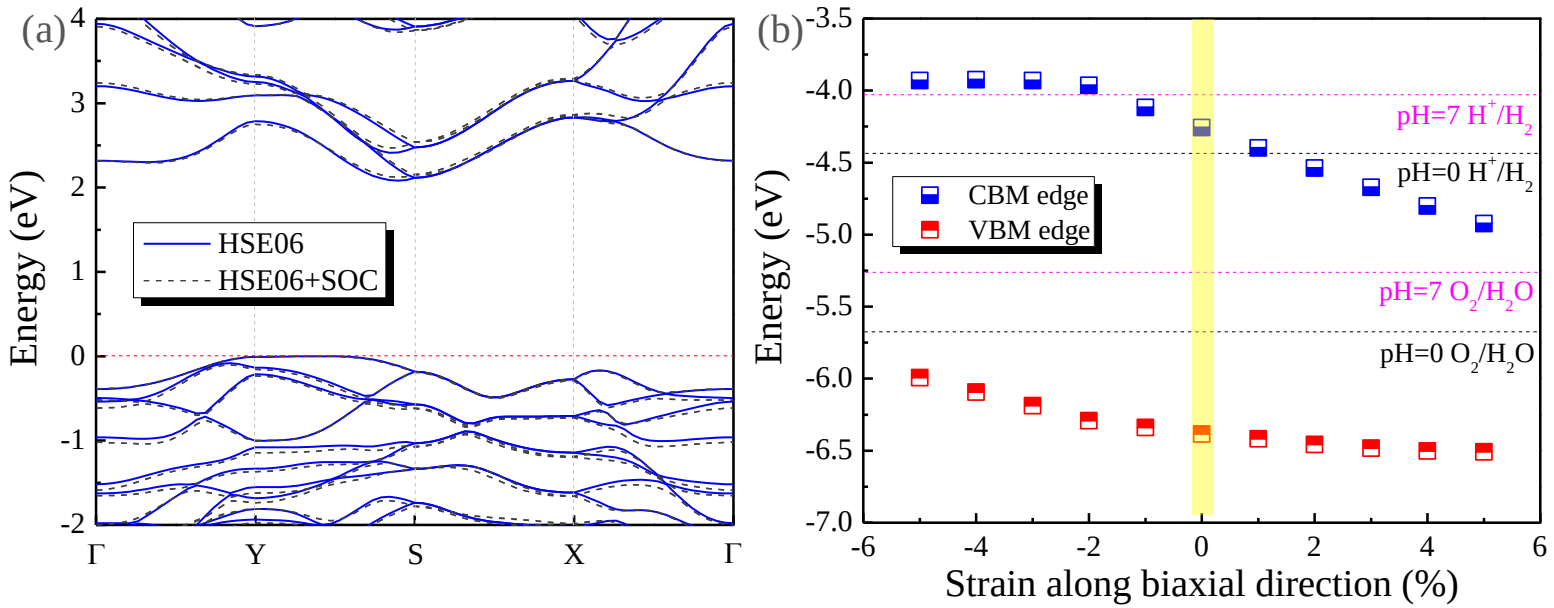
Indirect semiconductor with band gap of 2.12 eV

PdPS monolayer



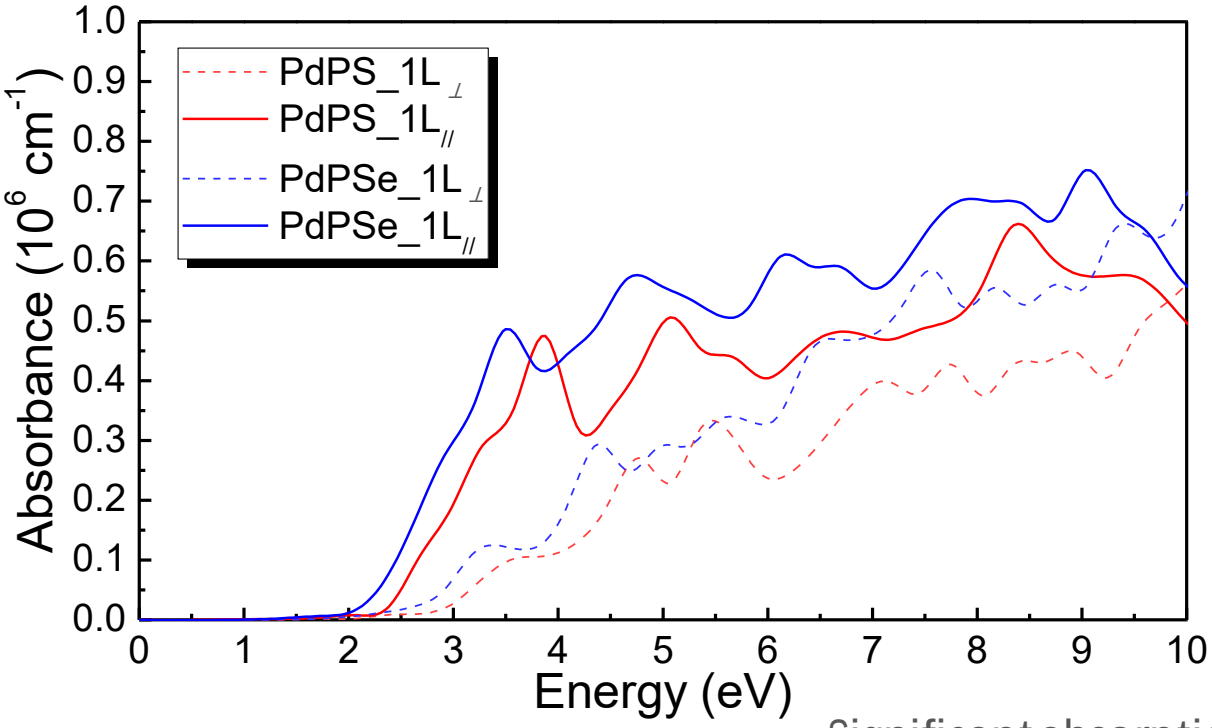
Band structure engineering by elastic strian

PdPSe monolayer



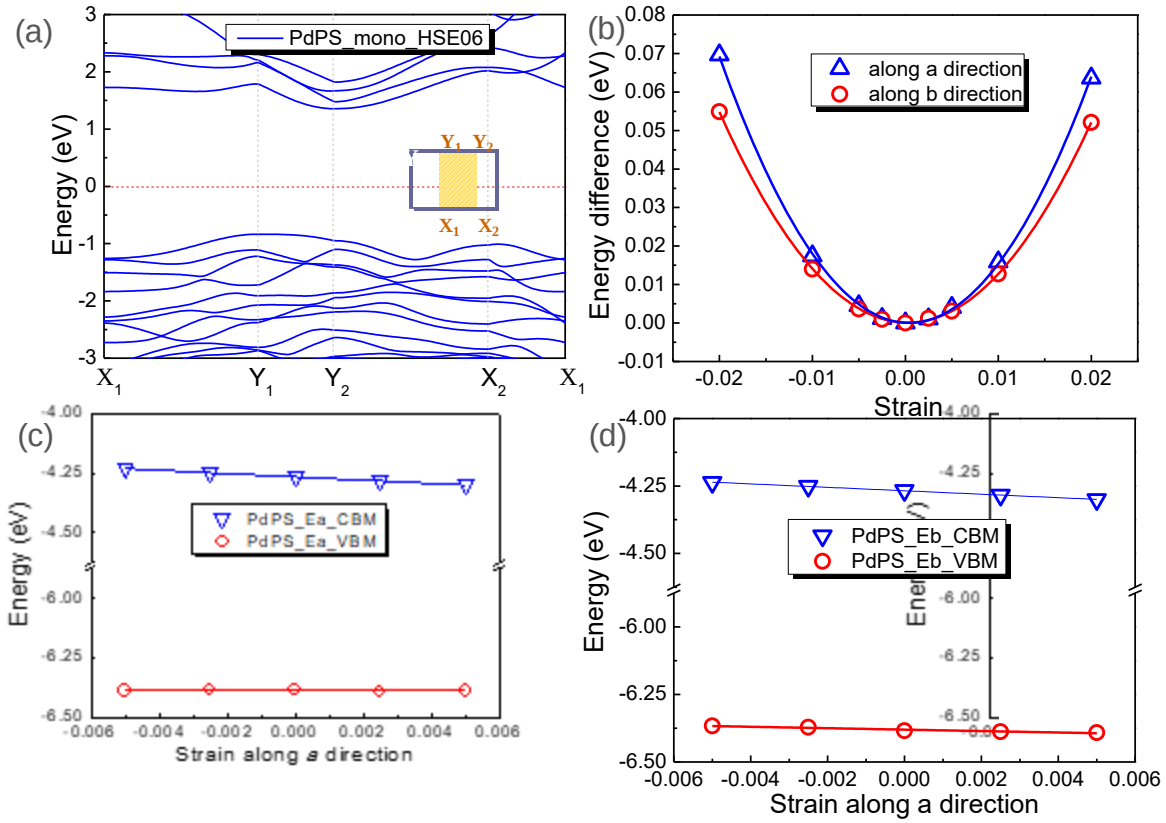
Indirect semiconductor with band gap of 1.97 eV

Light harvesting



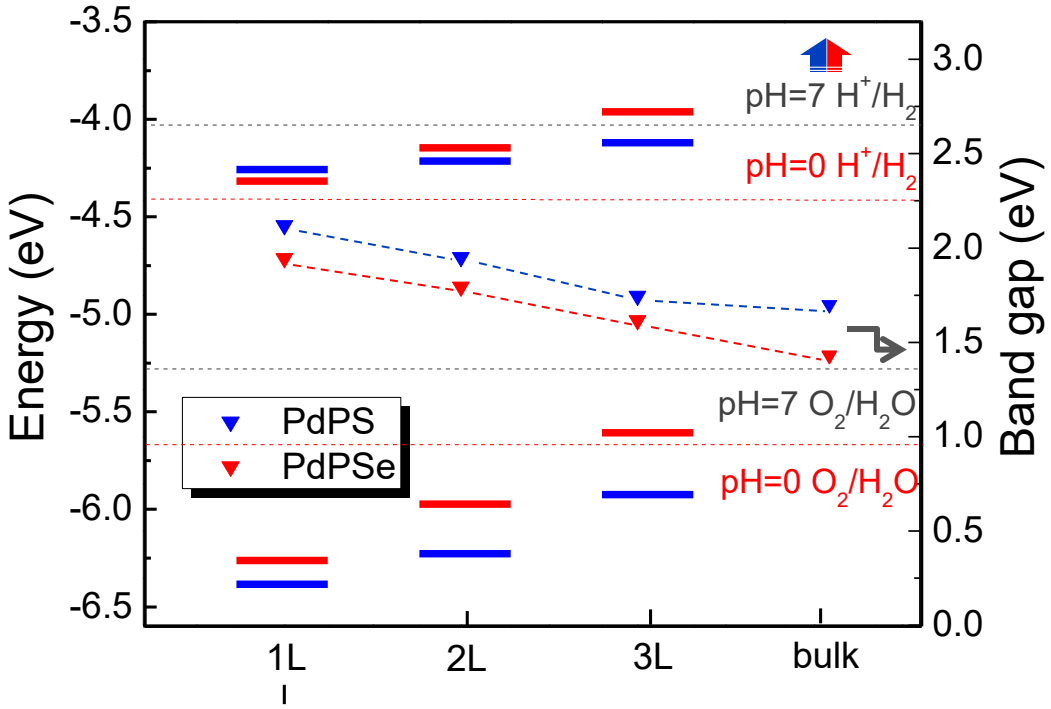
Significant absorption for visible light

Anisotropic carrier mobility



$cm^2 V^{-1} s^{-1}$	PdPS	PdPSe
electron_*a*	312	197
hole_*b*	249	344

Quantum confinement effects

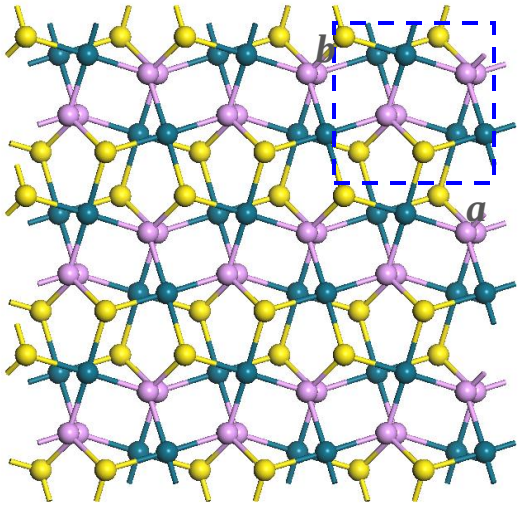


variation of electronic properties with increasing the layer thichness

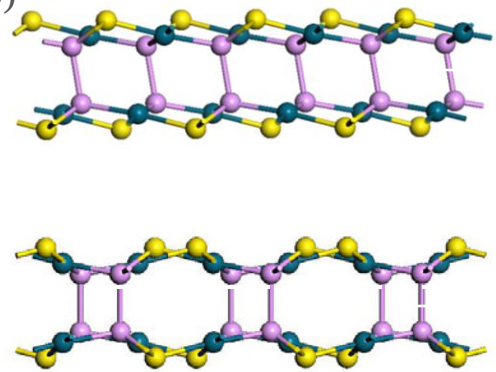
PdPX Conclusion

- Two novel two dimensional structures PdPS and PdPSe
- small cleavage energy and high stabilities
- Semiconductors with indirect band gap of ~ 2 eV
- High and anisotropic carrier mobility
- Pronounced light absorption
- Appropriate band edge for water splitting

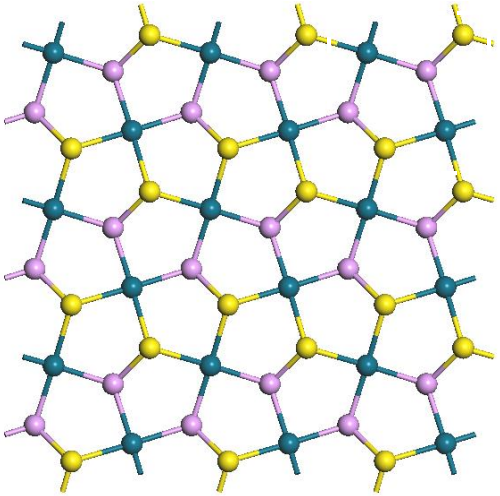
(a)



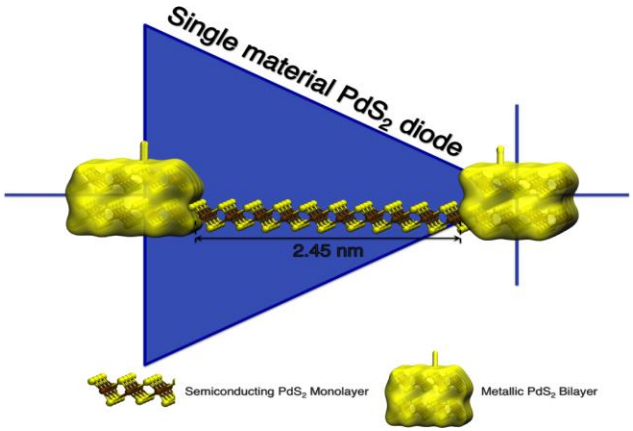
(b)



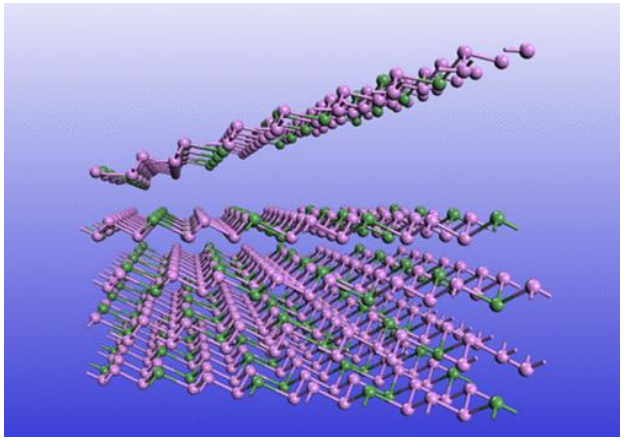
(c)



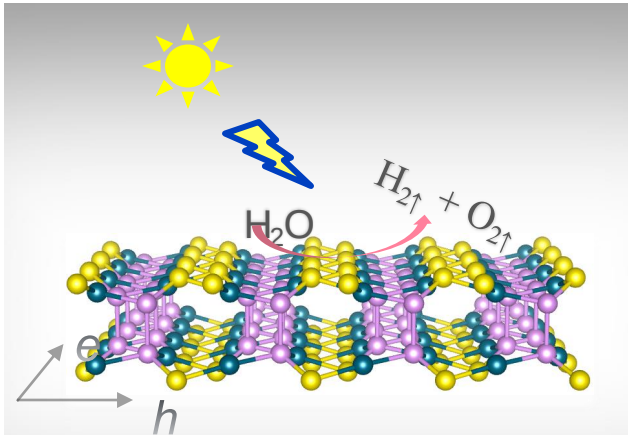
Summary



Group 10 metal dichalcogenides



2D electronics/optoelectronics: GeP_3



PdPX - photocatalysts

thomas.heine@uni-leipzig.de

Bonus track

Haeckelite NbS_2 two-dimensional crystal – a diamagnetic high mobility semiconductor with Nb4+ ions

Yandong Ma, Yu Jing, Agnieszka Kuc and Thomas Heine

Angewandte Chemie (in press)

„Allotropes“ of MoS_2?

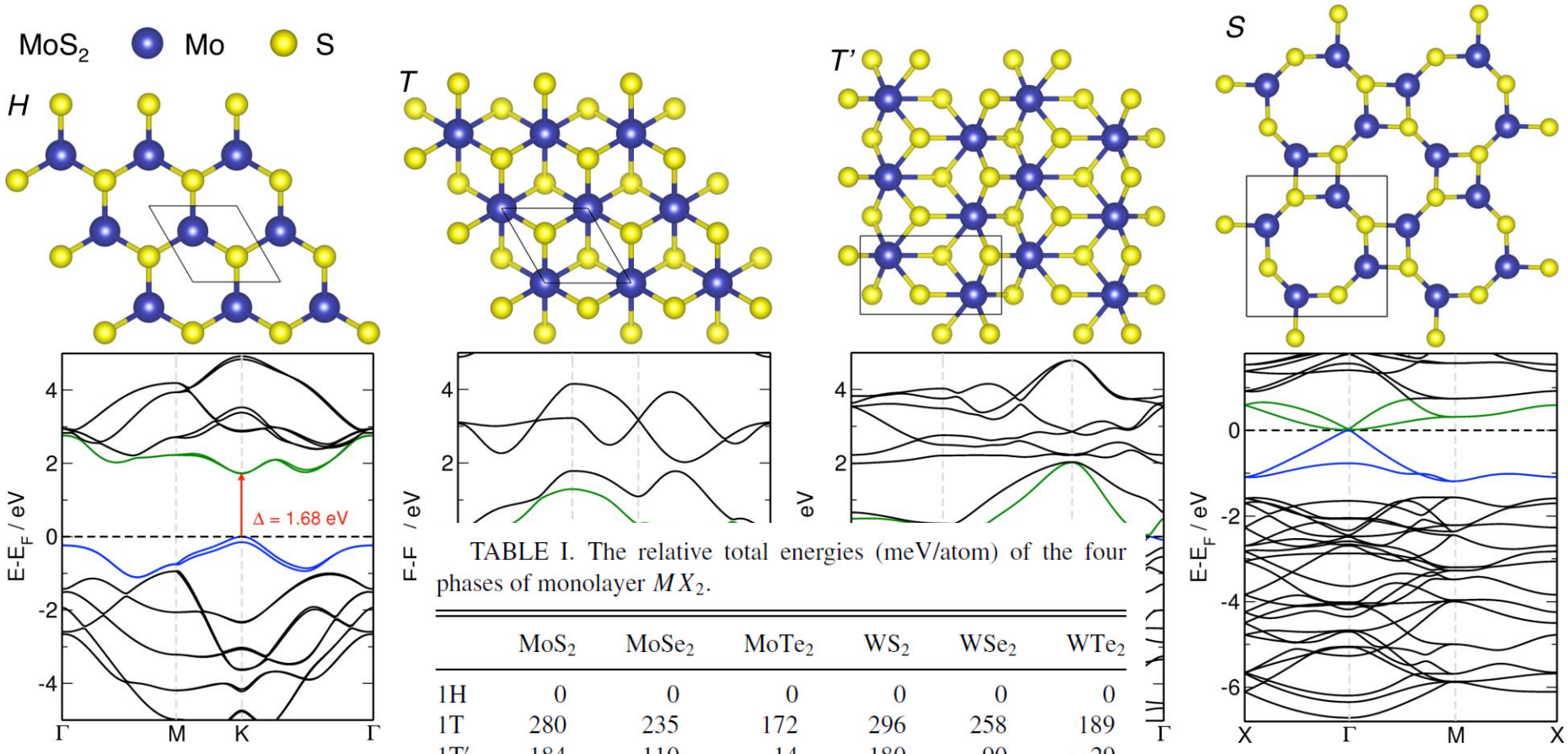
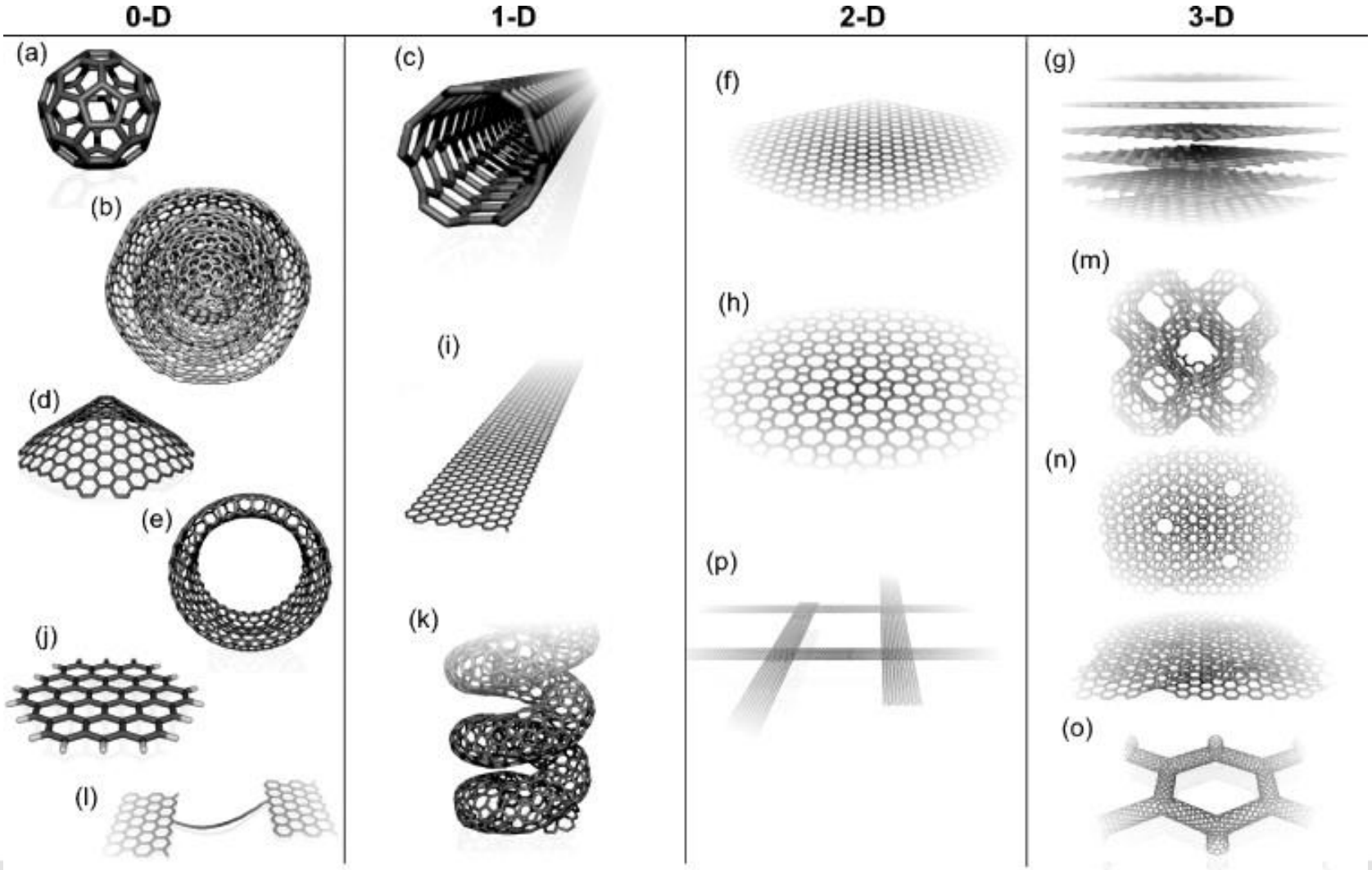


TABLE I. The relative total energies (meV/atom) of the four phases of monolayer MX_2.

	MoS_2	$MoSe_2$	$MoTe_2$	WS_2	WSe_2	WTe_2
1H	0	0	0	0	0	0
1T	280	235	172	296	258	189
1T′	184	110	14	180	90	−29
1S	286	243	183	326	268	181

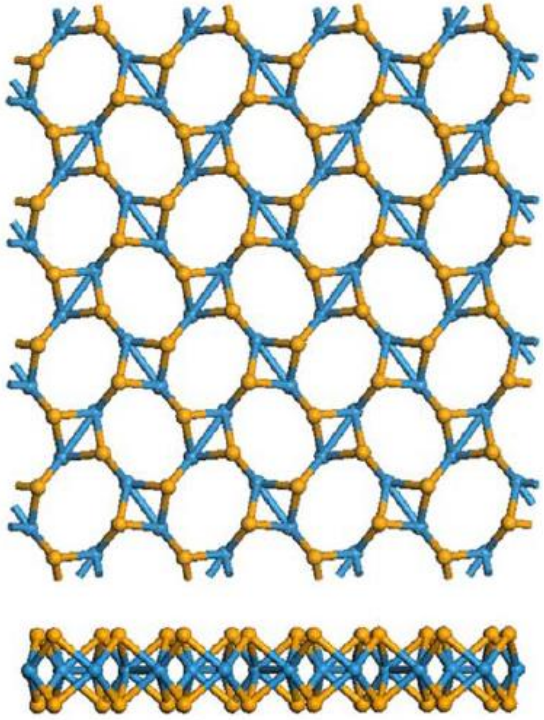
Y. Ma, L. Kou, X. Li, Y. Dai, S.C. Smith, T. Heine,
Phys. Rev. B 92 (2015) 085427.

Allotropes of carbon



M. Terrones, A. R. Botello-Méndez, J. Campos-Delgado, F. López-Urías, Y. I. Vega-Cantú, F. J. Rodríguez-Macías, A. L. Elías, E. Muñoz-Sandoval, A. G. Cano-Márquez, J.-C. Charlier, H. Terrones, nanotoday 5 (2010) 351-372.

Haeckelite Group 5 TMDC

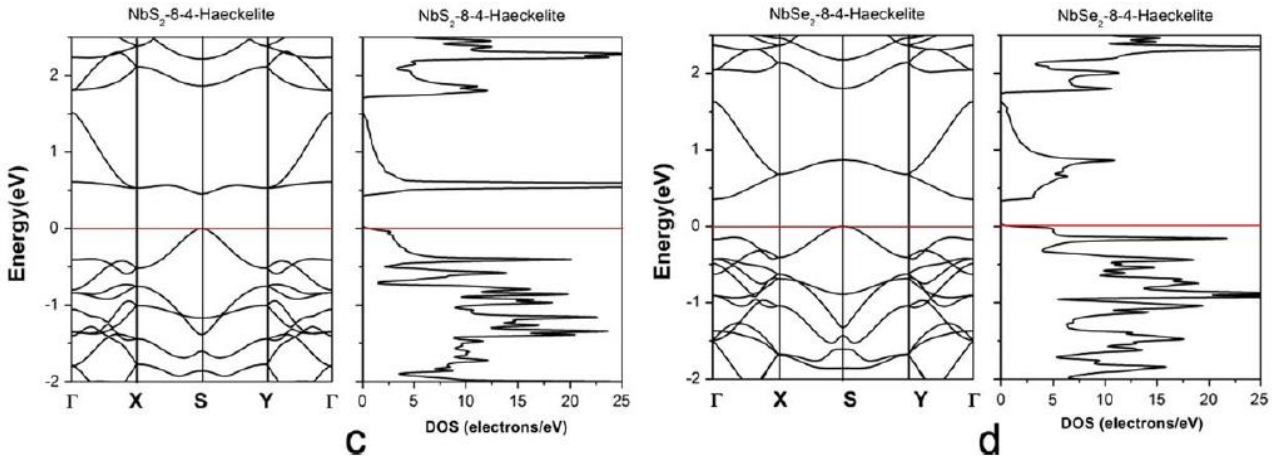


2D Materials

Letter

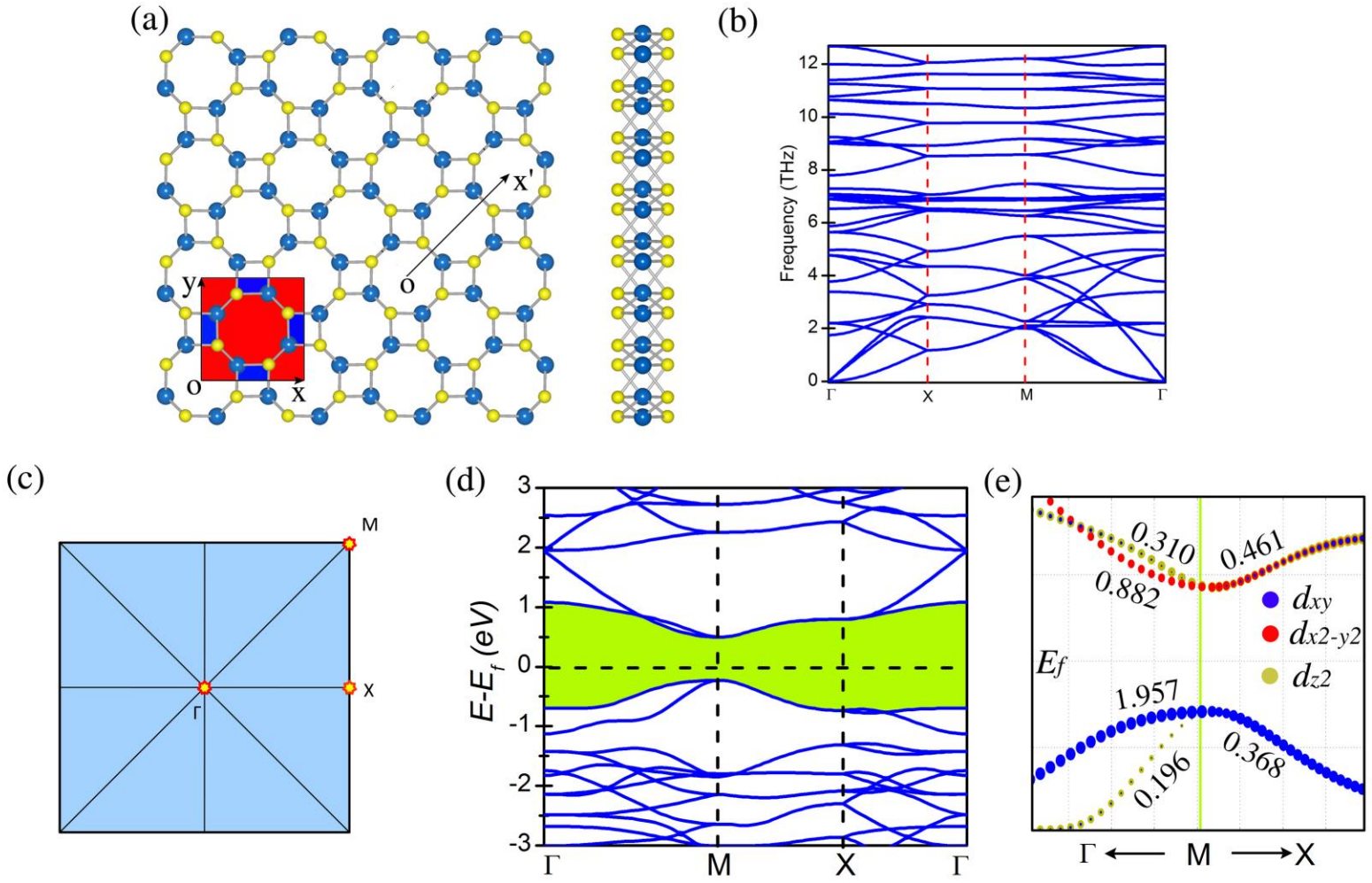
Electronic and vibrational properties of defective transition metal dichalcogenide Haeckelites: new 2D semi-metallic systems

H Terrones[1,4] and M Terrones[1,2,3]

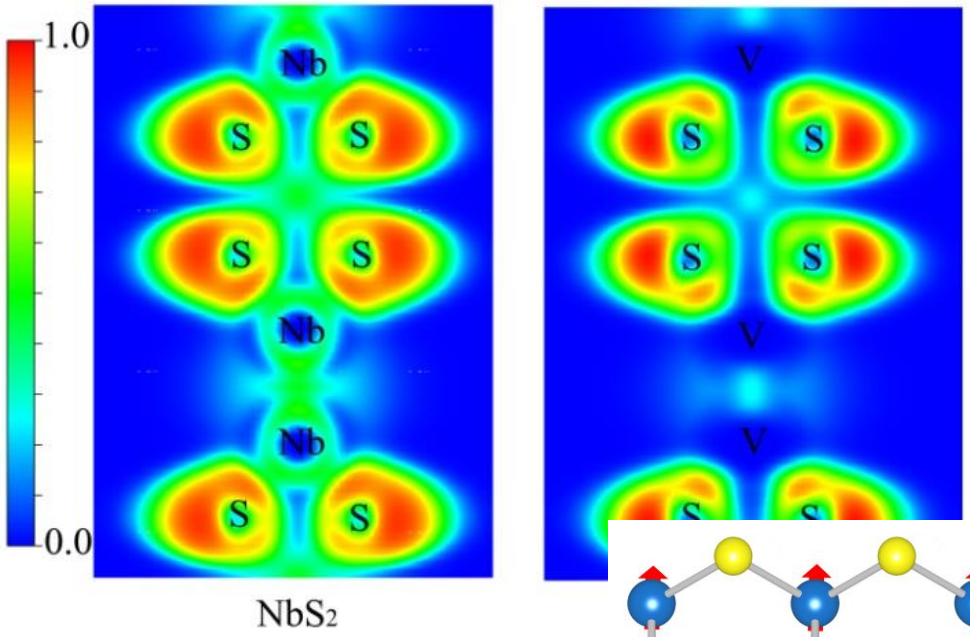


H. Terrones, M. Terrones, 2D Mater. 2014, 1, 011003

Haeckelite NbX_2 (X = S, Se, Te)



Diamagnetic S-NbX_2 (X = S, Se, Te)

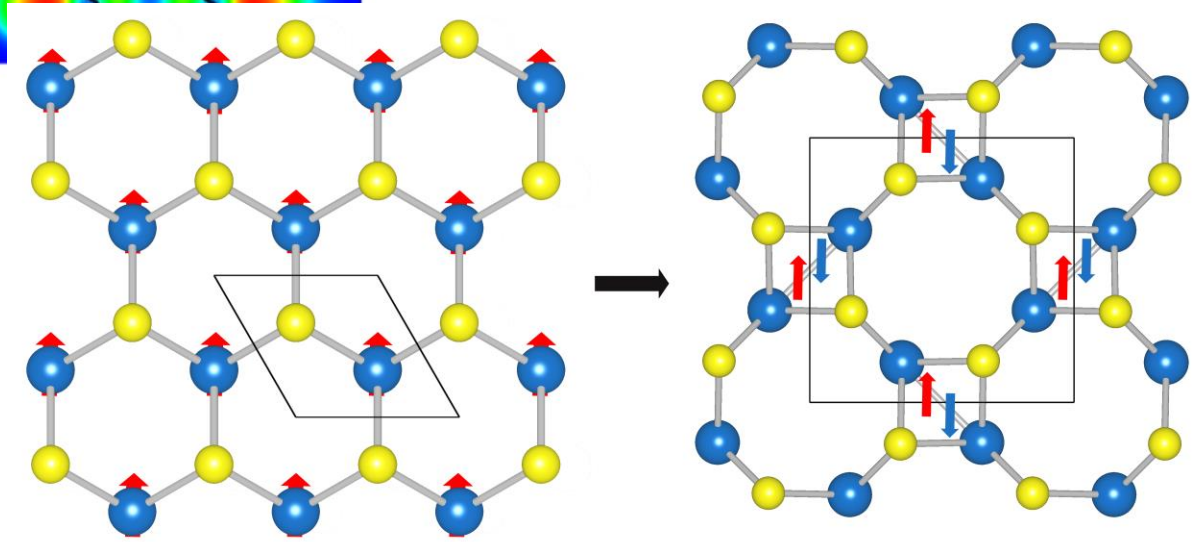


NbX_2: intermetallic bond pairs electrons

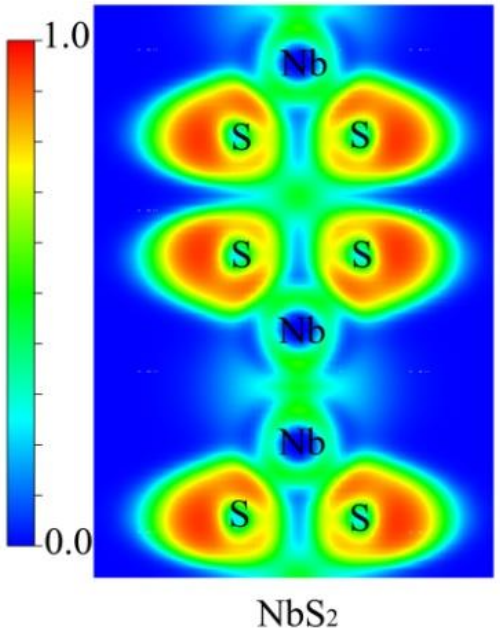
VX_2: localised electrons carry local spins

H-NbS_2: ferromagnetic

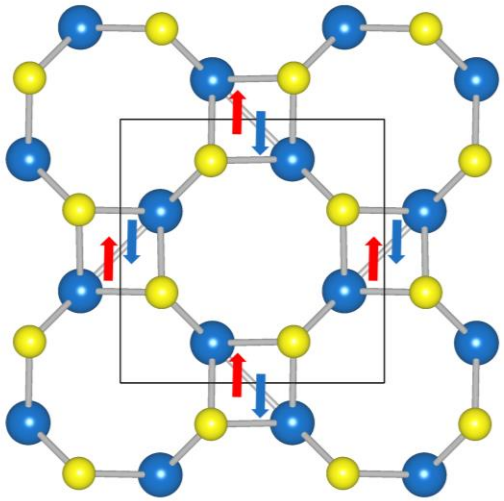
S-NbS_2: diamagnetic



Diamagnetic S-NbS_2



NbS_2



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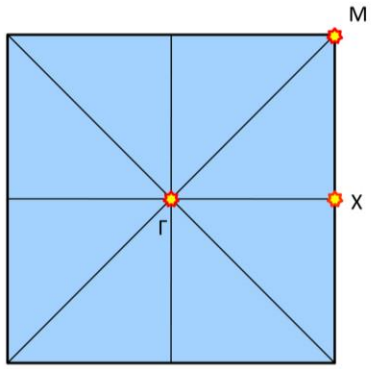
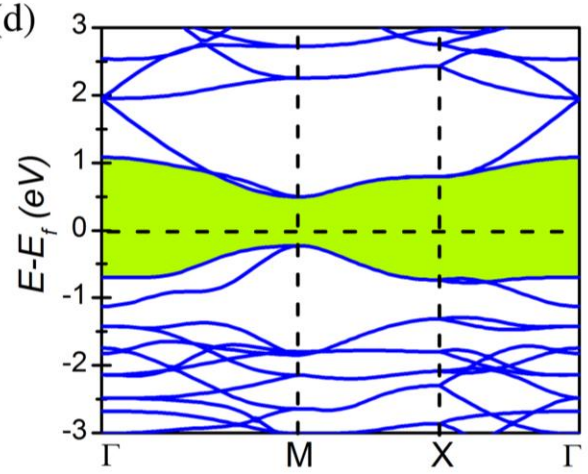


(d)



	NbS_2
Band gap (eV)	0.73
m_h/m_0	0.20…0.37
m_e/m_0	0.31…0.46
μ_h (10^2 $cm^2V^{-1}s^{-1}$)	1.3…4.9
μ_e (10^2 $cm^2V^{-1}s^{-1}$)	1.1…3.0

Methods

- k-space integration: Monkhorst-Pack
- Geometry optimization: PBE
- Electronic structure: HSE06 (or PBE0)
- Codes: ADF/BAND (numerical basis functions, explicit 2D boundary conditions) / VASP (repeated slab)
- Relativistic inertial mass (ZORA)
- Spin-Orbit coupling (collinear approximation)
- Phonons: harmonic approximation
- Effective masses: numerical from band structure
- Mobilities: deformation potential theory