# **2D Crystals for Science and Applications**



Prices on products are available upon request and depend on various factors such as cost of production, quality, dimensions, etc. Request to: <a href="mailto:nzhigadlo@gmail.com">nzhigadlo@gmail.com</a> <a href="https://crystmat.com">https://crystmat.com</a>

# **Black Phosphorus**



b-P bulk crystals grown at high pressure





Crystal structure of b-P

Ref.: <u>Nanoscale 2019, 11(39), 18449-18463</u> http://crystmat.com

# Black b-AsP



Crystal structure and EDX analysis of b-AsP crystal



b-AsP are semiconductors with tunable electronic and optical properties via tuning chemical compositions during material synthesis. May find unique applications in electronic and optoelectronic devices operate at infrared regime. Ref.: Nanoscale 11 (2019) 18449-18463

## **Elemental 2D materials: Tellurium**







Library of elemental 2D materials Encycl. of Nanomat. (2023) 1, 138-153 Crystal structure of multilayer tellurene. Red area represents a monolayer. J. Hazard.Mat. 423 (2022) 127148

# **Graphite and Graphene**



## Hexagonal boron nitride hBN



## MnP

## Potential 2D material for fundamental physics & electronic applications



# $Pd_xP_y$



Optical image of "Pd<sub>x</sub>P<sub>y</sub>" 2D crystals



Compounds in the Pd-P system Ref.: <u>Dalton. Trans. 42, 12667 (2013)</u>

Reactions of Pd with various amounts of P are efficient route to convert them into corresponding Pd phosphides  $Pd_xP_{y^*}$  Synthesis of crystalline PdP have proved to be very challenging.

# **2D Semiconductor GeAs**

Could outperform Si-based systems in terms of speed and energy efficiency



Used: optoelectronics, solar cells, sensors, radars, integrated circuits, quantum computingRef.: J. Cryst. Growth 631 (2024) 127627https://crystmat.com

## MnAs



### XRD with (h00) lines and SEM image





## MnAs has potential for exfoliation into thin layers

MnAs crystals exhibit a plate-like morphology with flat surfaces. J. Cryst. Growth 480 (2017) 148-153

MnAs is intriguing material because of its unique magnetic properties, phase transitions, and potential for use in cutting-edge technology like spintronics, thermoelectrics, and quantum computing.

### https://crystmat.com



First-order phase transition of MnAs

## InAs



Two-dimensional (2D) InAs is a promising for future electronic and optoelectronic applications such as nanoscale transistors, flexible and wearable devices, broadband photodetectors, heterogeneous integration with Si-based electronics.

# In(As,P)



Atom %

9.58

43.53

46.89

100.00

Element

Line

ΡК

As K

In L

Total

Weight

%

3.32

36.47

60.21

100.00

Weight %

+/-0.35

+/-1.69

+/-1.53

Error



In(As,P): (Cubic, F-43m, 216)

Key points: bandgap tuning, high-speed
electronics and optoelectronics, strain
engineering, temperature sensitivity,
integration with other materials

2D In(As,P) is a promising for future electronic and optoelectronic applications such as nanoscale transistors, flexible and wearable devices, broadband photodetectors, heterogeneous integration with Si-based electronics.

Atom %

+/- 1.02

+/-2.02

+/-1.19

Error

## **Classical antiferromagnet HoAs** Exhibit strong spin-orbit coupling & anisotropic magnetic interactions



Photo of HoAs crystals. It is unsuitable for exfoliation, yet its morphological appearance offers some hope.



HoAs is rock-salt structured and crystallizes in the cubic *Fm*-3*m* space group

The Neel temperature for HoAs is about 5 K, and the magnetic moments of Ho ions align in opposite directions in neighboring sublattices. Appropriate for studying electronic excited states, charge transport, and bonding interactions.

# Magnetic Topological Semimetal HoSb





Ho

Optical image of HoSb sample

HoSb crystallizes in NaCl structure with space group Fm-3m and orders AF at ~ 5.7 K

HoSb shows extremely large magnetoresistance (XMR). The Berry phase extracted from Shubnikov-de Haas oscillation indicates the possible nontrivial electronic structure of HoSb in the presence of magnetic field. HoSb offers a unique platform for exploring the interplay between XMR, magnetism and topology in an AFM matrix.

Ref.: Phys. Rev. B 98 (2018) 045137 ; Sci. Rep. 10, 12961 (2020) ; wikipedia

# **Topological semimetal InBi**





InBi (Tetragonal, P4/nmm, 129)

Key points: narrow bandgap, high mobility, strong spin-orbit coupling, quantum effects, thermoelectric applications

Extremely large positive magnetoresistance was found in a nonmagnetic semimetal InBi. Provides a new material platform for study of exotic topological quantum phases.

Ref.: Phys. Rev. B 108, 205107 (2023); New J. Phys. 19, 065007 (2017)

# NbS



## SEM image of NbS crystal

Element	Weight	Weight %	Atom	Atom %
Line	%	Error	%	Error
S K	32.20	+/- 0.79	57.92	+/- 1.42
Nb K	67.80	+/- 4.87	42.08	+/- 3.02
Total	100.00		100.00	
PDV	1.	CNIC	. 1	

#### EDX analysis of NbS crystal





Nice morphological appearance with 6-fold rotational symmetry

Phase Hor	Homogeneity	Chemical formula of	Structure	Space group	Lattice constants, A			
	range, at. %	sulfide and its formation temp., °C			а	b	С	c/a
NbS	54,54–47.367	NbS <sub>0.9</sub> >850 NbS <sub>1.2</sub> <850	Hexagonal	P6 <sub>3</sub> /mmc P6 <sub>3</sub> /mmc	3,33 3,32		6,39 12,92	1,1919 2×1,946

Information about NbS is very limited. Possibly suitable for exfoliation. Ref.: Poroshkovaya Metallurgiya, 11(35), 9-14, (1965) https://crystmat.com PbS

Possibly suitable for creation of thin layers via mechanical exfoliation



Optical image of PbS sample



PbS crystallizes in NaCl–type structure (cubic *Fm*-3*m*)

PbS is a semiconductor with a bandgap around 0.41 eV. This small bandgap allows it to absorb and emit infrared light, making it useful in IR detectors and optoelectronic devices.

Key interesting points: providing a playground for fundamental studies in condensed matter physics, electron-phono interactions, thermoelectric performance, photophysics and photochemistry, plasmon-exciton coupling, infrared optoelectronics, solar cells.

## NiS



Optical image of NiS crystals





Crystal structure of NiS



NiS crystallizes in trigonal R3m space group. Ni<sup>2+</sup> is bonded to five S<sup>2-</sup> atoms to form NiS<sub>5</sub> bipyramids.

NiS has two polymorphs. The  $\alpha$ -phase has a hexagonal unit cell, while the  $\beta$ -phase has a rhombohedral cell. Ref.: <u>Wikipedia</u>

# **2D Semiconductor GeS**

Versatile and exciting material for academic research and applications



Image of GeS thin flakes captured through the quartz glass ampoule wall



GeS: orthorhombic *Pnma* space group. Structure similar to black phosphorus

**Key Properties:** Two-dimensional layered structure, Direct band gap, High electron mobility, Strong photoluminescence, Good conductivity, Nonlinear optical properties

**Potentially useful** for next-generation high-speed electronics and optoelectronic devices, transistors, where thin, flexible, or even transparent materials are desirable

## **2D Semiconductor GaSe** Relevant for fundamental science and technological innovations



Element	Weight	Weight %	Atom
Line	%	Error	%
Ga K	48.37	+/- 0.62	51.48
Se K	51.63	+/- 1.01	48.52
Total	100.00		100.00

**Key points:** 1. Layered structure, 2. Nonlinear optical properties, 3. Wide bandgap, 4. Strong light-matter interaction, 5. High carrier mobility, 6. Photovoltaic & thermoelectric potential, 7. Quantum & topological effects, 8. Potential for heterostructures, 9. Mechanical flexibility

## PbSe



Optical image of PbSe samples



PbSe crystallizes in a NaCltype structure (cubic, *Fm*-3*m*)

PbSe is a semiconductor material. It has a direct bandgap of 0.27 eV at room temperature. It is used for manufacture of infrared detectors for thermal imaging, operating at wavelengths between 1.5–5.2 µm. Ref.: <u>wikipedia.org</u>

Key areas of interest: high-performance electronics, thermoelectric performance, infrared plasmonic devices (IR sensors, detectors, modulators), plasmon-exciton coupling, solar cells, transistors and flexible electronics, light-emitting diodes.

# Topological semimetal HgSe

Exhibit topologically nontrivial Weyl semimetal physics





### HgSe belongs to space group *F*-43*m*

Key Properties: direct bandgap, high carrier mobility, strong spin-orbit coupling, thermoelectric performance, infrared sensitivity, photoconductivity

HgSe is a promising material for potential applications in various fields such as electronics, spintronics, thermoelectrics, quantum computing and laser technologies.

## ZnSe

Attractive for applications in flexible and transparent nanoelectronic devices



Optical image of ZnSe samples

and Gd and X = 0, S, Se, and Te) chalcogenides. (b) BZ and projected surface BZ for (0001) surface of wurtzite MX chalcogenides.

By employing first-principles calculations it was predicted the existence of type-II Weyl phonons in ZnSe, a well-known II-VI semiconductor.

Ref.: J. Mater. Chem. A 2, 17971 (2014); Phys. Rev. B 103, 094306 (2021) https://crystmat.com

# Topological semimetal HfP<sub>2</sub>

Potential material for emerging optoelectronic and photovoltaic applications



Optical image of  $HfP_2$  crystals grown by chemical vapor transport method using iodine as transport agent.



 $HfP_2$  crystallizes in the orthorhombic structure with space group *Pnma* (No 62).  $Hf^{4+}$  is bonded in a 9-coordinate geometry to nine  $P^{2-}$  atoms.

**ARPES** data show direct observation of topological states in nodal-loop semimetal HfP<sub>2</sub>. Ref.: <u>Phys. Rev. Mater. 4, 054201 (2020)</u>.

First principles study predicting HfP<sub>2</sub> monolayer as promise candidate for photovoltaic water splitting and produce hydrogen fuel. Ref.: <u>RSC Adv. 12, 11202 (2022)</u>

## 2D Semiconductor GeAs<sub>2</sub> Promising candidate for thermoelectric applications

GeAs<sub>2</sub>





GeAs<sub>2</sub> crystallizes in the orthorhombic structure with the space group *Pbam* (No 55).

GeAs<sub>2</sub> is a 2D semiconductor with low thermal conductivity and high thermoelectric efficiency. Exfoliation of single-layer GeAs<sub>2</sub> is highly feasible and could be carried out by mechanical cleavage. Band-gap: bulk (0.99 eV), monolayer (1.64 eV).

# Topological semimetal ZrAs<sub>2</sub>





Optical image of ZrAs<sub>2</sub> crystalline samples

ZrAs<sub>2</sub> crystallizes in orthorhombic crystal structure (PbCl<sub>2</sub>, C23)

ZrAs<sub>2</sub>'s topological nature, nodal-line semimetal behavior, high carrier mobility, and potential for quantum phenomena make it a highly intriguing material for researchers studying new types of quantum states.

ZrAs<sub>2</sub> exhibits large magnetoresistance properties, it offers a new platform for unveiling interesting physics beyond Weyl semimental and topological insulator systems. Ref.: <u>Phys. Rev. B 110, 035142 (2024)</u>; <u>B 110, 054114 (2024)</u>

# NbAs<sub>2</sub>

NbAs<sub>2</sub> belongs to a large family of transition metal dipnictides MPn<sub>2</sub> (M = V, Nb, Ta, Cr, Mo, and W, Pn = P, As and Sb).



Magnetoresistance of NbAs<sub>2</sub>, elemental metals and other binary compounds.



NbAs<sub>2</sub> crystallizes in a monoclinic system with the centrosymmetric space group of C12/m1.

### Ref.: Phys. Rev. Mat. 2 (2018) 024203

Ref.: <u>Sci. Rep. 8 (2018) 6414</u>

NbAs<sub>2</sub> exhibit extremely large magnetoresistance at low temperatures, which is ascribed to an effect for compensation of electrons and holes with large mobilities.

Ref.: Phys. Rev. B 93 (2016) 195119; Phys. Rev. B 93 (2016) 184405 https://crystmat.com

## LaBi<sub>2</sub>





Optical image of LaBi<sub>2</sub> sample

Resistance of  $LaBi_2$  as a function of T and P

LaBi<sub>2</sub> reveals metallic behavior without indications of magnetic ordering. Superconductivity appears at high pressure, but its origin is not clarified yet. Ref.: <u>Phys. Rev. Materials 3, 095006 (2019)</u>

Key points of interest: combination of topological properties, strong spin-orbit coupling, potential for Majorana fermions, thermoelectric applications, quantum computing, spintronic devices, transistors, sensors, energy harvesting.

# 2D Semiconductor MoS<sub>2</sub>

MoS<sub>2</sub> plays an important role in condensed matter physics research



Optical image of  $MoS_2$  single crystals. 2D  $MoS_2$  monolayers can be produced by exfoliating bulk crystals.  $MoS_2$ : hexagonal  $P6_3/mmc$  space group. Monolayer is a layer of Mo atoms sandwiched between two layers of S atoms.

Bulk MoS<sub>2</sub> has an indirect gap of 1.2 eV. MoS<sub>2</sub> monolayers have a direct gap of 1.8 eV. Under an electric field MoS<sub>2</sub> monolayers have been found to superconduct at 9.4 K.

Applications: Field-effect transistors; Photodetectors; Solar cells; Chemical sensors; Supercapacitors & batteries; Spintronics; Valleytronic devices.

# NbS<sub>2</sub>



Crystal structure of NbS<sub>2</sub>

Superconducting transition of  $NbS_2$ 

 $NbS_2$  can be exfoliated into ultrathin grayish sheets similar to other transition metal dichalcogenides. These layers exhibit superconductivity, where the transition temperature increases from ca. 2 to 6 K with the layer thickness increasing from 6 to 12 nm, and then saturates with thickness.





Optical image of PtS<sub>2</sub> sample



 $PtS_2$  crystallizes in the *P*-3*m*1 space group of the trigonal system. Ref.: <u>Wikipedia</u>

PtS<sub>2</sub> semiconductor: bandgap of 0.25 eV for bulk and 1.6 eV for monolayers

Key points of interest: 2d layered material, semiconductor, spin-orbit coupling, topological properties, high carrier mobility, thermal stability, catalysis potential, form heterostructures, flexible nanoelectronics, quantum devices.

PtSe<sub>2</sub>



PtSe<sub>2</sub> crystal possesses a 1T-type hexagonal crystal structure with P-3m1 space group, as show in Fig. (a) and (b).

 $PtSe_2$  is semimetallic, but when reduced to few layers it becomes a semiconductor. The band gap is calculated as 1.2 eV for monolayer, and 0.2 eV for bilayers. For a trylayer or thicker the substance loses a bandgap and becomes semimetalic.

Monolyers of  $PtSe_2$  show helical spin texture, which is not expected for centrosymmetric materials such as this. This property could be due to a local dipole induced Rashba effect. It means that  $PtSe_2$  is a potential spintronics material. Ref.: <u>Wikipedia</u>

# 2D Layered NbSe<sub>2</sub>

NbSe<sub>2</sub> is fascinating material because of its layered structure, superconductivity, charge density wave phase, and capacity to host topologically intriguing states.



Weight % Err.	Atom %	Atom % Err.	
+/- 1.18	65.49	+/- 1.25	NDSe <sub>2</sub> : $P6_3/mmc$ space grou
+/-3.10	34.51	+/-2.79	Ref.: 2D Mater. 3 (2016) 0350
,	100.00	,,	

6) 035028

https://crystmat.com

Element

Se K

Nb K

Total

Weight %

61.73

38.27

100.00

# 2D Semiconductor ReSe<sub>2</sub>

May exhibit novel quantum states under strain, electric or magnetic fields, such as exotic phases or topologically protected edge states



Possible applications: in flexible and stretchable electronics, optoelectronics, and thermoelectrics (photodetectors, sensors, lasers, transistors, displays).

100.00

Total

100.00





Optical image of NiSe<sub>2</sub> sample



 $NiSe_2$  crystallizes in orthorhombic *Pbca* space group.  $Ni^{2+}$  is bonded to 6 Se<sup>1-</sup> atoms to form  $NiSe_6$  octahedra.

 $NiSe_2$  can be exfoliated into 2D layers. Exhibit much better catalytic performance than well-studied  $MoS_2$  and  $WS_2$ -based catalysts.

NiSe<sub>2</sub> key interesting points: promising topological and thermoelectric material, superconductivity, catalytic activity (alternative to Pt-based catalysts in fuel cells and batteries), creating heterostructures with other 2D materials.

## MoTe<sub>2</sub> Material for numerous functionalities



Applications of MoTe<sub>2</sub>: Energy storage (batteries, supercapacitors), catalysis, sensors, solar cells, photodetectors, field-effect transistors, etc.

Error Line Error 28.08 34.18 MoL +/-0.46 +/-0.56 Te L 71.92 +/-0.7165.82 +/-0.65 Total 100.00100.00

 $MoTe_2$  sheets can be thinned down to monolayers that are flexible and almost transparent. Mechanically adjustable and opto-electronically tunable  $MoTe_2$  has potential for wearable and flexible electronic devices. Ref.: <u>Wikipedia</u>

# 2D Semimetal HfTe<sub>2</sub>



Element Weight Weight % Atom Atom % Line % % Error Error Te L 58.82 66.65 +/- 0.81 +/-0.92 Hf L 41.18 +/-0.9833.35 +/- 0.80 Total 100.00 100.00



Optical image of HfTe<sub>2</sub> single crystals



HfTe<sub>2</sub> key points: layered structure and topological characteristics, candidate for Weyl semimetal, strong spin-orbit coupling, anomalous magnetoresistance, possible superconductivity, tuning via strain & dimensionality, potential for thermoelectrics.

# 2D Semimetal WTe<sub>2</sub>

Material for cutting-edge science

Image of WTe<sub>2</sub> crystals

Crystal structure of WTe<sub>2</sub>

EDX analysis of WTe<sub>2</sub>



WTe<sub>2</sub> is a type-II Weyl semimetal. Bulk crystal reveals large magnetoresistance and pressure-driven superconductivity. Electrons in a WTe<sub>2</sub> flake can exhibit hydrodynamic behaviour, exhibiting traits similar to those of classical fluids.

Refs.: <u>Wikipedia</u> ; <u>Nat. Physics 17 (2021) 1216</u>

## FeTe<sub>2</sub>

Material with promises for applications that relatively unstudied experimentally



FeTe<sub>2</sub> was synthesized from high purity elements employing evacuated silica tube technique. Specimen was heated, reground and annealed at 450 °C several times until complete.



FeTe<sub>2</sub> crystallizes in orthorhombic structure with space group *Pnnm*. Cooling down to 2 K, paramagnetic to AF and then FM phase transitions were observed at 79 K and 35 K.

Ref.: J. Phys.: Condens. Matter 32, 035808 (2020); ACS Omega 6, 10537 (2021)

# 2D Semiconductor $\alpha$ -HgI<sub>2</sub>



HgI<sub>2</sub> is a semiconductor for construction of X- and  $\gamma$ -ray detectors for digital medical imaging. HgI<sub>2</sub> has a wide optical band-gap (2.1 eV) and high photon absorption coefficient for high-energy radiation.

## YbGa<sub>2</sub> Predicted as potential topological electronic material



Optical image of YbGa<sub>2</sub> crystals



Hexagonal P6\_3/mmc space group

YbGa<sub>2</sub> key aspects: Yb valence state, potential for quantum criticality and superconductivity, magnetic properties, heavy fermion behavior, quantum technologies, low-dimensionality, electronic band structure, high pressure effects

At pressure above 22 GPa, YbGa<sub>2</sub> undergoes structural phase transition and Yb increase oxidation state from 2+ to 3+. Ref.: <u>ZAAC 627, 2249 (2001)</u>

# $Bi_2S_3$

 $Bi_2S_3$  has lamellar structure and can be exfoliated down to monolayers through standard mechanical exfoliation technique.



Image of Bi<sub>2</sub>S<sub>3</sub> crystals

Crystal structure of Bi<sub>2</sub>S<sub>3</sub>

 $Bi_2S_3$  is crystallized in orthorhombic structure (space group *Pnma*) and has semiconducting behaviour with band gap ~1.3 eV and large absorption coefficient of 105 cm-1. Interesting candidate for thermoelectrics, photodetectors, solar cells and supercapacitors.

 $Sb_2S_3$ 

### Topological insulator, high mobility 2D semiconductor



Optical image of Sb<sub>2</sub>S<sub>3</sub> crystal



Sb<sub>2</sub>S<sub>3</sub> crystallizes in orthorhombic structure, space group *Pbnm* (a = 11.23 Å, b = 11.31 Å, c = 3.84 Å, Z = 4). Ref.: <u>Wikipedia</u>

 $Sb_2S_3$  is a promising photovoltanic material. With band gap of 1.7-1.8 eV it has been considered as a perfect component for top sub cell in Si-based tandem solar cells. Ref.: Nat. Commun. **10**, 4540 (2019); Joule **2**, 857-878 (2018)

# 2D topological insulator Bi<sub>2</sub>Se<sub>3</sub>



Bi<sub>2</sub>Se<sub>3</sub> is an intriguing material due to its topological insulating properties, potential for quantum computing, spintronic applications, and thermoelectric capabilities. Its distinct electronic structure and 2D surface states make it a crucial material for advancing both fundamental physics and cutting-edge technologies.

# 2D Topological insulator Sb<sub>2</sub>Te<sub>3</sub>



Key interesting points: thermoelectric, quantum computing, spintronics, lasers, infrared detectors, non-volatile memory, data storage technology.

# 2D Topological insulator Bi<sub>2</sub>Te<sub>3</sub>

 $Bi_2Te_3$  is a topological insulator. It is an efficient thermoelectric material for refrigeration or portable power generation. The layers are stacked together via van der Waals interactions and can be exfoliated into thin 2D layers.



An idealized band structure for a topological insulator. Fermi level falls within bulk band gap which is traversed by topologicallyprotected spin-textured Dirac surface states.

Ref.: Ann. Rev. Cond. Mat. Phys. 2: 55 (2011)



 $Bi_2Te_3$  crystallizes in a rhombohedral structure with the space group *R-3m*, and is described by a hexagonal unit cell.

Ref.: Sci. Rep. 9: 10790 (2019)

# Au<sub>2</sub>Te<sub>3</sub>

Heavy elements such as Au and Te have potential to form compounds with strong spin-orbit coupling and narrow band gaps. Little is known about  $Au_2Te_3$  compound.



Te atoms form octahedra around Au atoms, creating displaced double layers

Ref.: Wikipedia; Science 145 (3632), 581-583 (1964); Nat Phys Sci 231, 67-68 (1971)

https://crystmat.com

+/- 0.92

+/- 1.05

60.67

39.33

100.00

49.98

50.02

100.00

+/- 0.76

+/-1.33

Te L

Au L

Total

# 2D Helimagnet ferric chloride FeCl<sub>3</sub>



Optical image of FeCl<sub>3</sub> single crystals



FeCl<sub>3</sub>: hexagonal structure *R*\_3, No 148

A neutron diffraction study found a helimagnetic structure for  $FeCl_3$  below 15 K. A field induced magnetic transition was also observed in  $FeCl_3$ .

### Ref.: Crystals 7 (2017) 121

 $FeCl_3$  layers can be intercalated with graphite. This van der Waals system combines frustration and disorder, due to intercalation, and may be hosting topologically non-trivial magnetic phases. Ref.: Phys. Rev. B 105 (2022) 054418

# Bi<sub>2</sub>Se<sub>2</sub>S



Image of Bi<sub>2</sub>Se<sub>2</sub>S sample



The crystal structure of the tetradymite  $M_2Xe_2Y$ 

### Ref.: New J. Phys. 13, 095005 (2011)

The ternary tetradymite-like compouds  $M_2Xe_2Y$  (M = Bi or Sb; X and Y = S, Se or Te) are variations of binary compounds  $Bi_2Se_3$  and  $Bi_2Te_3$ . They are predicted to have an isolated Dirac cone on their naturally cleaved surface.

# 2D topological insulator $Sb_{2,1}(Te_{0.95}S_{0.05})_{2,9}$



Element	Weight	Weight %	Atom	Atom %
Line	%	Error	%	Error
S K	1.17	+/- 0.07	4.41	+/- 0.27
Sb L	41.64	+/- 1.17	41.37	+/- 1.17
Te L	57.19	+/- 1.65	54.22	+/- 1.56
Total	100.00	-	100.00	



 $Sb_{2.1}(Te_{0.95}S_{0.05})_{2.9}$  crystallizes in rhombohedral structure with *R*-3*m* space group. Ref.: Nanoscale Res. Lett. 16, 22 (2021)

Key interesting points: thermoelectric, quantum computing, spintronics, lasers, infrared detectors, non-volatile memory, data storage technology.

# $HgTe/Sb_2Te_3 = Sb_{2.8}Hg_{0.2}Te_{3.95}$ Perspective topological insulator material



Optical image of  $Sb_{2.8}Hg_{0.2}Te_{3.95}$  crystalline sample Mutual solubility of HgTe and  $Sb_2Te_3$  is insignificant

# 2D Semiconductor BiSeBr

Offers a new avenue for research, spintronic applications & quantum computing



Key properties: Topologically protected surface states (Dirac fermions, quantum spin Hall effect), strong spin-orbital coupling, high-temperature stability, layered structure.

## BiSeI

Topological Insulator • Thermoelectric • Quantum Computing & Spintronics



### Optical image of BiSeI single crystals

Element	Weight	Weight % Atom %		Atom %
Line	%	Error		Error
Se K	19.25	+/- 0.82	33.65	+/- 1.43
ΙL	30.45	+/- 0.65	33.12	+/-0.71
Bi L	50.31	+/- 1.51	33.23	+/- 0.99
Total	100.00		100.00	-

EDX analysis of a single crystal BiSeI



BiSeI crystallizes in orthorhombic *Pnma* space group. It can be exfoliated into thin layers. J. Cryst. Growth 517 (2017) 7-11

Application: solar cells, photodetectors, thermoelectrics, catalysis, sensors, LEDs, nonlinear optics, lasers, LEDs

Key points of interest: tunability of bandgap, ultrathin thickness, intrinsic anisotropic characteristics, potential for integration with metal oxide semiconductors.

# Non-superconducting Na<sub>x</sub>CoO<sub>2</sub>

Quasi-2D material consisting of triangular 2D  $CoO_2$  layers with Na atoms in between



space group

Na<sub>x</sub>CoO<sub>2</sub> key points: superconductivity and thermoelectric properties, unique crystal structure, strong correlations, sodium intercalation (tunability), energy storage and battery applications, potential for new phases and new physics.

# 2D non-superconducting FeTe<sub>0.65</sub>Se<sub>0.35</sub>



Optical image of FeTe<sub>0.65</sub>Se<sub>0.35</sub> single crystals grown under high pressure



Crystal structure of FeTe<sub>0.65</sub>Se<sub>0.35</sub>

Crystal structure of FeTe<sub>0.65</sub>Se<sub>0.35</sub> demonstrating tetrahedral coordination of Fe1 ions in 2a positions by anions of Se and Te and interstitial Fe2 ions in 2c position in anion plane. Atoms in Fe2 position are at interstitial sites between Te/Se atoms. Fe1 atoms are itinerant, Fe2 type atoms are localized with a magnetic moment of 2.5  $\mu_B$  and are destructive for superconductivity.

Homogeneous  $FeTe_{0.6}Se_{0.4}$  crystals without excess of Fe2 and without variation in composition is non-superconducting. Ref.: J. Cryst. Growth 432 (2015) 95

# 2D Janus compound PtSeTe



PtSSe PtSTe PtSeTe

 $PtS_2$ 

PtSe<sub>2</sub>

PtTe<sub>2</sub>

Photos of PtSeTe polycrystalline samples

From PtX<sub>2</sub> monolayers to Janus PtXY

PtSeTe can be interesting for band enginnering, sensors, optoelectronics, valleytronics, memory devices, transistors, topological transition, Rasha effect. Ref.: J. Phys.: Condens. Matter 30, 245502 (2018); Nanoscale Adv. 3, 6608 (2021)

# KInS<sub>2</sub>





Optical image of KInS<sub>2</sub> samples

 $KInS_2$  crystallizes in the monoclinic space group C2/c. The bonding is highly covalent and exhibits both 2D and 3D features.

Limited information on the physical properties of KInS<sub>2</sub> is available. It has a bandgap of 3.0 eV. Ref.: J. Solid State Chem. 92, 2, 520-530 (1991)

# 2D Cuprate Bi<sub>2</sub>Sr<sub>2</sub>CuO<sub>6+x</sub>



Optical images of  $Bi_2Sr_2CuO_{6+x}$  crystals

Bi2201 is simpler than its relatives like Bi2212 and Bi2223 because it only contains a single  $CuO_2$  layer between Bi-based layers, making it a model system for studying the role of these planes in the superconducting mechanism.



 $Bi_2Sr_2CuO_{6+x}$ 

# 2D Superconductor Bi<sub>2</sub>Sr<sub>2</sub>CaCu<sub>2</sub>O<sub>8+x</sub>



Optical image of Bi2212

Laue diffraction patterns of  $Bi_2Sr_2CaCu_2O_{8+x}$  crystals



Quasi 2D cuprate Bi2212 provide insights into mechanisms of superconductivity Ref.: Nat. Commun. 5, 5708 (2014); J. Phys.: Condens. Matter 6, 8969 (1994) https://crystmat.com

## YBa<sub>2</sub>Cu<sub>4</sub>O<sub>8</sub>



Superconductor without oxygen ordering in chains & with fixed oxygen stoichiometry. ARPES allows separately investigate electronic properties of  $CuO_2$  planes and CuO chains. Ref.: Phys. Rev. Lett. 98, 157002 (2007); Phys. Rev. B 90, 140501 (2014)

## Pt0



Optical image of PtO sample



PtO crystallizes in tetragonal symmetry with P4/mmc space group

PtO key points: catalysis, hydrogenation reactions, hydrogen storage, fuel cells, precursor for Pt nanoparticles, thermal stability, photocatalysis, electronic devices.

Experimental data for PtO is very limited and contradicted. Doubts remain even for bulk PtO structures. Ref.: <u>Phys. Rev. B 84, 100101(R) (2011)</u>

# 2D Mica Mineral





A rock with mica from Canton of Ticino, Switzerland



Schematic view of mica crystal structure



Mica has a wide band gap of 5 eV, great thermal and chemical resistance, making it an excellent insulating substrate for heterogeneous 2D material structures.

Ref.: Nanotechnology 19, 305705 (2008) Sci. Reports 12, 14076 (2022)

## CaSiO<sub>3</sub>





# Optical image of Wollastonite – calcium silicate mineral $CaSiO_3$

The unit cell of triclinic CaSiO<sub>3</sub>. This formula may also be written as Ca(Si<sub>3</sub>O<sub>9</sub>)<sub>0.33</sub> or as Ca<sub>3</sub>(Si<sub>3</sub>O<sub>9</sub>).

Canadian Wollastonite is a little-known a relatively rarely-occuring mineral with a pearly luster on cleavage surfaces and a granular texture. Ref.: <u>Wikipedia.org</u>