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: nzhigadlo@gmail.com https://crystmat.com

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_xP_y" 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 _{0.9} >850 NbS _{1.2} <850	Hexagonal	P6 ₃ /mmc P6 ₃ /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. Ni²⁺ is bonded to five S²⁻ atoms to form NiS₅ bipyramids.

NiS has two polymorphs. The α -phase has a hexagonal unit cell, while the β -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 HfP₂

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 HfP₂. Ref.: <u>Phys. Rev. Mater. 4, 054201 (2020)</u>.

First principles study predicting HfP₂ monolayer as promise candidate for photovoltaic water splitting and produce hydrogen fuel. Ref.: <u>RSC Adv. 12, 11202 (2022)</u>

2D Semiconductor GeAs₂ Promising candidate for thermoelectric applications

GeAs₂





GeAs₂ crystallizes in the orthorhombic structure with the space group *Pbam* (No 55).

GeAs₂ is a 2D semiconductor with low thermal conductivity and high thermoelectric efficiency. Exfoliation of single-layer GeAs₂ is highly feasible and could be carried out by mechanical cleavage. Band-gap: bulk (0.99 eV), monolayer (1.64 eV).

Topological semimetal ZrAs₂





Optical image of ZrAs₂ crystalline samples

ZrAs₂ crystallizes in orthorhombic crystal structure (PbCl₂, C23)

ZrAs₂'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.

ZrAs₂ 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>

NbAs₂

NbAs₂ belongs to a large family of transition metal dipnictides MPn₂ (M = V, Nb, Ta, Cr, Mo, and W, Pn = P, As and Sb).



Magnetoresistance of NbAs₂, elemental metals and other binary compounds.



NbAs₂ 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>

NbAs₂ 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

LaBi₂





Optical image of LaBi₂ sample

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

LaBi₂ 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 MoS₂

MoS₂ 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 MoS₂ has an indirect gap of 1.2 eV. MoS₂ monolayers have a direct gap of 1.8 eV. Under an electric field MoS₂ monolayers have been found to superconduct at 9.4 K.

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

NbS₂



Crystal structure of NbS₂

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 PtS₂ sample



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

PtS₂ 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.

PtSe₂



PtSe₂ 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 NbSe₂

NbSe₂ 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 ₂ : $P6_3/mmc$ 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 ReSe₂

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 NiSe₂ sample



 $NiSe_2$ crystallizes in orthorhombic *Pbca* space group. Ni^{2+} is bonded to 6 Se¹⁻ 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.

NiSe₂ 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.

MoTe₂ Material for numerous functionalities



Applications of MoTe₂: 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 HfTe₂



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 HfTe₂ single crystals



HfTe₂ 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 WTe₂

Material for cutting-edge science

Image of WTe₂ crystals

Crystal structure of WTe₂

EDX analysis of WTe₂



WTe₂ is a type-II Weyl semimetal. Bulk crystal reveals large magnetoresistance and pressure-driven superconductivity. Electrons in a WTe₂ flake can exhibit hydrodynamic behaviour, exhibiting traits similar to those of classical fluids.

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

FeTe₂

Material with promises for applications that relatively unstudied experimentally



FeTe₂ was synthesized from high purity elements employing evacuated silica tube technique. Specimen was heated, reground and annealed at 450 °C several times until complete.

FeTe₂ 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 α -HgI₂

HgI₂ is a semiconductor for construction of X- and γ -ray detectors for digital medical imaging. HgI₂ has a wide optical band-gap (2.1 eV) and high photon absorption coefficient for high-energy radiation.

YbGa₂ Predicted as potential topological electronic material

Optical image of YbGa₂ crystals

Hexagonal P6_3/mmc space group

YbGa₂ 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, YbGa₂ 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 Bi₂S₃ crystals

Crystal structure of Bi₂S₃

 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 Sb₂S₃ crystal

Sb₂S₃ 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 Bi₂Se₃

Bi₂Se₃ 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 Sb₂Te₃

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

2D Topological insulator Bi₂Te₃

 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)

Au₂Te₃

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 FeCl₃

Optical image of FeCl₃ single crystals

FeCl₃: 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

Bi₂Se₂S

Image of Bi₂Se₂S 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_xCoO₂

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

space group

Na_xCoO₂ 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_{0.65}Se_{0.35}

Optical image of FeTe_{0.65}Se_{0.35} single crystals grown under high pressure

Crystal structure of FeTe_{0.65}Se_{0.35}

Crystal structure of FeTe_{0.65}Se_{0.35} 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 μ_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

PtSe₂

PtTe₂

Photos of PtSeTe polycrystalline samples

From PtX₂ 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)

KInS₂

Optical image of KInS₂ 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 KInS₂ is available. It has a bandgap of 3.0 eV. Ref.: J. Solid State Chem. 92, 2, 520-530 (1991)

2D Cuprate Bi₂Sr₂CuO_{6+x}

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 Bi₂Sr₂CaCu₂O_{8+x}

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

YBa₂Cu₄O₈

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)

CaSiO₃

Optical image of Wollastonite – calcium silicate mineral $CaSiO_3$

The unit cell of triclinic CaSiO₃. This formula may also be written as Ca(Si₃O₉)_{0.33} or as Ca₃(Si₃O₉).

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>