

## Physical properties

### Magnetic properties

Antiferromagnetism	Magnetization relaxation
Diamagnetism	Magneto-striction
Ferrimagnetism	Magneto-structural correlations
Ferromagnetism	Magnetocaloric effect
Hysteresis	Magnetoelectric properties
Itinerant ferromagnetism	Magnetoresistance
Magnetic anisotropy	Multiferroic
Magnetic coupling	Paramagnetism
Magnetic dilution	Quantum tunneling of magnetization (QTM)
Magnetic dynamics	Quantum spin liquid (QSL)
Magnetic entropy	Spin canting
Magnetic exchange interactions	Spin frustration
Magnetic moment	Spin transition
Magnetic ordering	Spin-chain systems
Magnetic phases	Spin-ladder systems
Magnetic refrigeration	Spin-Polarization
Magnetic structure	Superparamagnetism
Magnetic susceptibility	Temperature-induced excited spin state trapping (TIESST)
Magnetization	Weak ferromagnetism
Magnetization dynamics	

### Electrical properties

Dipole moment	Ionic conductivity
Electrical conductivity	Magnetoelectric properties
Electrical resistivity	Paraelectricity
Electrocaloric effect	Piezoelectricity
Electrochemical properties	Proton conductivity
Electroluminescence	Pyroelectric properties
Ferroelectricity	Semiconductor
Hall effect	Superconductivity
Hall resistivity	Thermoelectric properties

### Optical properties

Alexandrite effect	Optical activity
Birefringence	Phosphorescence
Chromogenic recognition	Photoactivation
Chromophoric properties	Photochromic behavior
Chromotropic behaviour (colour change upon heating or grinding)	Photoluminescence (PL)
CIE chromaticity coordinates	Reflectivity
Energy level diagram	Refractive index
Fluorescence	Second harmonic generation (SHG)
Luminescence	Transparency
Mechanochromic behavior	Triboluminescence (TL)
Non-linear optical response	Two-photon-excited fluorescence spectroscopy (2PEF)

### Mechanical properties

Bulk modulus	Lattice dynamics
Compressibility	Piezoelectricity
Elastic constants	Shape memory materials
Elastic properties	Thermoelastic properties
Flexible crystals (strain:reversible deformation)	Vickers hardness
High-pressure structural transformations	

### Thermal properties

Anisotropic thermal expansion	Thermal conductivity
Heat capacity	Thermal expansion
Lattice expansion	Thermal stability
Negative thermal expansion	Thermochromism
Seebeck effect	Thermoelectric properties
Specific heat	

### Physicochemical properties

Catalytic activity	Mixed valence
Electrochemical properties	Molecular orbital diagram
Energy profiles	Reactivity
Energy transfer	Sensitivity toward impact and friction
Interaction coefficients	Stability constants
Kinetic parameters	Thermodynamic properties

## Dielectric properties

AC electrical conductivity	Dielectric constant
DC electrical conductivity	Dielectric permittivity
Dielectric relaxation	Nyquist plots

## Applied methods

### Spectroscopic methods

Dielectric spectroscopy	NQR
Electron spin resonance spectroscopy (ESR)	Nuclear resonance vibrational spectroscopy (NVRS)
Electronic absorption spectra	Raman
Electronic absorption/emission spectra	Resonant ultrasound spectroscopy (RUS)
Electronic excitation/emission spectra	Time-resolved optical spectroscopy
Elemental analysis (ICP-OES)	Ultrafast transient absorption spectroscopy
Energy-dispersive spectroscopy (SEM-EDS)	UV-vis
EPR spectroscopy	UV/vis optical absorbance spectra
EXAFS	UV/vis-NIR emission spectroscopy
Femtosecond spectroscopy	UV/vis-NIR reflectance spectroscopy
FT-IR	UV/vis-NIR spectroscopy
Impedance spectroscopy	X-ray absorption spectroscopy (XAS)
IR	X-ray photoelectron spectroscopy (XPS)
Moessbauer spectroscopy	XANES
NMR spectroscopy	

### Calculation methods

ab initio calculations	Molecular dynamics analysis (MD)
Band structure	Molecular orbital calculations (MO)
Bond-valence sums (BVS)	Monte Carlo calculations
Computational studies	Natural bond orbital analysis (NBO)
Crystal field calculations	Natural localized molecular orbital analysis (NLMO)
DFT	QTAIM calculations
Electronic structure calculations (e.g. DOS)	Quantum chemical theory (QCT) computations
Geometry optimization	Quantum-chemical calculations
Lattice energy calculations	TD-DFT
Ligand field theory (LFT)	Thermodynamic calculations

Machine-learning methods	Valence bond analysis
MAPLE calculations	

### Thermometry

Differential scanning calorimetry (DSC)	Thermal stability
Differential thermal analysis (DTA)	Thermogravimetry (TGA,TG)
Thermal analysis	

### Electrochemistry

Amperometry	Electrochemical sensing
Charge/Discharge curves	Potentiometry
Cyclovoltammetry (CV)	Redox properties
Differential pulse voltammetry (DPV)	Solid electrolytes

### Magnetometry

Annealing	SQUID magnetometry
Spin state	

### Microscopy

Atomic force microscopy (AFM)	High resolution transmission electron microscopy (HRTEM)
Contact Kelvin Probe Force Microscopy (cKPFM)	Piezoresponse force microscopy (PFM)
Electron backscatter diffraction (EBSD)	Scanning electron microscopy (SEM)
HAADF-STEM	Selected area electron diffraction (SAED)
High resolution electron microscopy (HREM)	Transmission electron microscopy (TEM)

### Crystal structure

(3+1)D super space group	Microstructure
Anion ordering	Modulated structure
Approximant structure	Nanoparticles (NP)
Atomic site preference	New mineral
Cation ordering	New structure type
CH- $\pi$ interactions	Non-covalent interactions
Chemical bonding	Order-disorder
Chirality	Overbonding
Coordination environment	Phase diagram
Coordination modes	Phase equilibria
Crystal packing	Phase evolution
Crystallography instrumentation	Phase separation

Disorder	Phase transition
Doping	pi-pi stacking interactions
Electron backscatter diffraction (EBSD)	Polar structure
Electronic structure	Polymer structure
Enantiomorphism, chiral structures	Polymorphism
Fourier maps	Polytypism
Framework structure	Quasicrystals
Glass-like transition	Rotation electron diffraction (RED)
Group-subgroup relationship	Satellite peaks
Hirshfeld surface analysis	Selected area electron diffraction (SAED)
Host-guest compounds	Single-crystal growth
Hydrogen bond interactions	Single-crystal to single-crystal transformation (SCSC)
Hydrolytic and thermal stability	Small-angle X-ray scattering (SAXS)
Incommensurate composite crystal structure	Solvatomorphism
Insulator-to-metal transition	Spin-orbit coupling (SOC)
Intercalation	Spinel inversion
Intermolecular interactions	Stacking variants
Interpenetrating networks	Structural evolution
Interstitial layers	Structure prediction
Interstitial site	Superflip refinement
Intramolecular interactions	Symmetry reduction
Jahn-Teller distortion	Topology
Layered structures	Twinning
Li+ intercalation	Vacancies
Lithiation	Van-der-Waals interactions
Long-range ordering	

### Chemical composition

Cation distribution	Phase diagram
Complex metallic alloys (CMA)	Phase transformation
Doping	Polar intermetallics
Electron micro probe analysis (EMPA)	Polyoxometalates (POM)
Electron-rich clusters	Postspinel phases
Energy-dispersive X-ray spectroscopy (EDX)	Solid solution

Heusler alloys	Solubility
Intermetallics	Superacids
Lattice expansion	Zeolites
Phase boundaries	Zintl phases

## Synthesis

Annealing	Modulation of properties: ligand configuration modes
Arc-melting	Modulation of properties: ligand conformation modes
Asymmetric synthesis	Modulation of properties: ligand coordination modes
Bridgman method	Modulation of properties: ligand electronic effects
Chemical vapor transport (CVT)	Modulation of properties: ligand steric effects
Chemical vapour deposition (CVD) (thin film production)	Modulation of properties: ligand transformation modes
Crystal growth	Modulation of properties: metal ion association modes
Czochralski method	Modulation of properties: protonation
Electrochemical synthesis	Modulation of properties: reagent concentration effects
Floating zone method	Photochemical synthesis
Flux-growth	Reaction coordinates
Hard and soft acids and bases concept (HSAB)	Reaction mechanism
High pressure synthesis	Self-assembly
HT-HP synthesis	Sol-gel route
Hydrothermal synthesis	Solid-state synthesis
Ionothermal synthesis	Solvent-modulation of the structure
Mechanochemical synthesis	Solvothermal synthesis
Modulation of properties: cation exchange effects	Synthesis, Molecular Structure, Reaction mechanisms
Modulation of properties: ligand bridging modes	

## Technical Application

### Optoelectronics

Chiroptical properties	Near-UV blue emission LEDs
Circularly polarized luminescence (CPL)	NLO materials
Deep-ultraviolet laser	OLED technology
Deep-ultraviolet transparent materials (DUV)	Optical fibers
Duplex switches	Phosphor
Electronic circular dichroism (ECD)	Photocurrent response materials

Field emission display (FED)	Proton recognition
Free space optical communication systems (FSO)	Scintillator(radiation detection)
Laser materials	Selective and sensitive metal cation detection
LED technology	White-light emission (WLE)
Light-emitting electrochemical cells (LEC)	

### Energy

Batteries, Electrode materials	Optical band gap
Capacitor materials	Photovoltaic
Dye-sensitized solar cells (DSSC)	Protonic ceramic fuel cells (PCFCs)
Energy storage systems	Scintillators
Energy storage: dehydration/rehydration	Semiconductor
Energy transformation and Data storage	Solar cells
Fuel cells	Solid electrolytes
Hydrogen evolution	Solid oxide fuel cells (SOFC)
Hydrogen storage	Superconductors
Lithium-ion conductor	Thermoelectrics

### Environmental properties

Actinide extraction	Determination of IO <sub>4</sub> (-) ions
Anion detection	Determination of MnO <sub>4</sub> (-) ions
Azo dyes degradation	Determination of Mo(6+)
Biodegradability	Determination of N <sub>2</sub> H <sub>2</sub>
Biodegradable polymers	Determination of P <sub>2</sub> O <sub>7</sub> (4-) ions
Cadmium immobilization	Explosives
CO <sub>2</sub> adsorption	Fluorescence sensor for bioactive ions (Pi detection)
CO <sub>2</sub> capture	Hg <sup>2+</sup> removal
CO <sub>2</sub> capturing during combustion of fuels (CLOU)	Ion exchange
CO <sub>2</sub> fixation/reduction	Ion extraction
Corrosion inhibition	Luminescent sensor for pesticides
Desulfurization of fuels	Nuclear fuel cycle
Detection of CO	Nuclear waste remediation
Detection of environmental pollutants	Organic dyes adsorption/decomposition
Detection of nitroaromatics	Phosphate capture
Detection of NO <sub>2</sub>	Plastic waste

Detection of $\text{UO}_2(2+)$ ions	Radioactive applications
Determination of $\text{CN}^-$ anions	Radionuclide waste disposal
Determination of $\text{Cr}_2\text{O}_7(-)$ ions	Rare-earth elements extraction
Determination of $\text{Cu}(2+)$ ions	Reduction of $\text{NO}$
Determination of $\text{Fe}(3+)$ ions	Sensor for organic molecules
Determination of $\text{Hg}^{2+}$ ions	

## Catalysis

Alcohol oxidation catalysts	Hydroalumination
Alkane oxidation catalysts	Hydroamination catalysts
Alkoxylation catalysts	Hydroboration catalysts
Alkylation catalysts	Hydroformylation catalysts
Alkynylation catalysts	Hydrogen transfer
Asymmetric catalysis	Hydrogenase catalysts
Bioinspired catalysis	Hydrogenation catalysts
Bond activation	Hydrolysis catalysts
C-N bond formation	Hydrosilylation catalysts
Carbon-heteroatom bond formation	$\text{N}_2$ fixation, $\text{N}_2$ activation
Catalyst precursors	$\text{N}_2$ reduction catalysts
$\text{CO}_2$ cycloaddition	$\text{N}_2\text{O}$ activation
$\text{CO}_2$ insertion	O-O bond cleavage
$\text{CO}_2$ reduction catalysts	$\text{O}_2$ activation
Cyanosilylation catalysts	OER catalysts (Oxygen evolution reaction)
Cycloaddition reactions	Orthometalation
Cycloalkene oxidation catalysts	Photocatalysis
Decarbonylation	Photoelectrochemical water-splitting
Dehydration of benzamides	Photoresponsive $\text{CO}$ release
Dehydrocoupling (DHC) of Phosphines	Polymerization catalysts
Dehydrogenation catalysts	Post-synthesis surface functionalization
Deoxygenation	Redox properties
Desulfurization of fuels	Separation of volatile organic compounds
Electrocatalytic activity	Stereoselective catalysts
Electrocatalytic $\text{H}_2$ oxidation	Stereospecific catalysts
Enantioselective catalysts	Sulfoxidation catalysts



Epoxidation catalysts	Transmetalation reactions
Gas absorption	Volatile organic compound (VOC) degradation
Gas separation	Water absorption
H <sub>2</sub> production	Water oxidation catalysts
HER catalysts (Hydrogen evolution reaction)	Water reduction
Heterogeneous catalysis, multifunctional catalysts	Water splitting catalyst

### Materials&Sciences

Absorbent materials	Magneto-optical materials
Anion extraction agents	Magnetofluids
Atomic layer deposition (ALD)	Molecular sieves
Bistability	Organic field-effect transistors (OFETs)
Data storage	Semimetallic oxides
Degradable packing materials	Shape memory materials
Diamond	Smart windows
Dielectrics	Smash-glow crystals
Dyes	Solar absorbers
Energy source	Solar filters
Ferroelectric field-effect transistors (FeFET)	Space applications
Ferroelectric random access memory (FeRAM)	Space applications
Gas Adsorption	Steel technology
High-energy density materials (HEDM)	Supercapacitor materials
Impact and damage sensors	Sustainable energy production
Ionic liquids	Thermoelectric materials
Luminescent thermometer	Thin film applications
Magnetic electrides	Tracers
Magnetic refrigeration technology	Zero-dimensional materials

### Nano

#### Nano structures

Co-crystallization	Nanomaterials
Core-shell structures	Nanoparticles (NP)
Nanocages	Nanorods
Nanocapsules	Nanosheets

Nanocluster	Nanospheres
Nanocrystals	Nanotubes
Nanodots (NDs)	Nanowires
Nanofibers	Pseudomorphic nanocrystal assemblies
Nanojars	Surface plasmon absorption

### Nano applications

Molecular nanomagnet	Nanoscale engineering
Nanoporous materials	

## Organometallics

### Structural description

0D structures	Layered structures
1D channel structures	Lewis acid-base complexes
1D coordination compounds	Ligand
2D networks	Long-range ordering magnets (LROs)
3D framework	Macrocycles
Anderson POM	Mesoporous materials
Asymmetric ligands	Metal-carbene framework (MCF)
Cage structures	Metal-HC interactions
Cavitands	Metal-metal bond
Cavity size effects	Metal-metal interactions
Chain structures	Metal-organic frameworks (MOF)
Channels, pores	Metal-organic macrocycles
Chelates	Metal-organic magnetic multilayers (MOMMs)
Chiral coordination compounds	Metallacrowns
Cluster compounds	Metallacycles
Configurational isomers	Metallaheteroboranes
Conformational isomers	Metallamacrocycles
Coordination polyhedra	Microporous materials
Coordination polymers (CPs)	Nanoporous materials
Cubane structures	Organometallic dendrons, dendrimers
Donor-acceptor interactions	Paddlewheel complex
Fullerenes	Polyoxometalates (POM)

Fulleride anions	Redox-induced conversions
Halogen bridging interactions	Secondary building units (SBU)
Helical structures	Self-assembly reactions
Heterometallic complexes	Structure-luminescence relationship
Host-guest interactions	Supertetrahedral clusters
Host-guest-systems	Supramolecular coordination complexes (SCCs)
Hybrid ligands	Supramolecular structures
Inorganic-organic hybrids	Template
Isomerism	Topological analysis
Keggin POM	Triple decker complexes
Large cavity structures	Zintl clusters

### Ligands

Acetates (ac)	Ligand symmetry - coordination
Acetylacetonates (acac)	Linker (Bridging Ligand)
Amide	Metallacycles
Azido complexes	Metallatranes
Bioactive NO complexes	Metallocenes
Bipyricorroles	Metallylenes
Bipyridines (bpy)	N-heterocyclic carbenes (NHC)
Bitetrazolates	N-heterocyclic silylenes (NHSis)
Carbazoles	NHC ligands
Carbido complexes	Nicotinates
Carbonyl	Oxamates
Carboranes	P/N ligands
Carboxylates	Phenantrolines (phen)
Catecholates	Phenylpyridines (ppy)
Chelates	Phosphines
Chinolines	Phthalocyanines
Chiral ligands	Pincer ligands
Chlorins	Pivalates
Coronates	PNP pincer ligands
Crown ethers	Porphyrins
Cryptand	Pyrazoles

Cyclopentadiene (Cp)	Pyridines
Diacylthiourea	Pyrimidines
Diaminopropane (dap)	Quinolines
Diimines	Redox-noninnocent ligands
Dithiocarbamates	Salicyl
Ditopic phosphonate ester	Schiff bases
Ethylenediamine (en)	Scorpionates
Fullerenes	Terpyridines
Halogen bonded adducts	Tetrazoles
Hyrido complexes	Thiobenzoates
Imidazoles	Thiolate
Imine	Thiosemicarbazones
Iodido complex	Triazoles
Ligand design	Triazolpropanamide (TPA)
Ligand isomerization	TTF derivatives
Ligand precursors synthesis	Weakly coordinating anions (WCA)
Ligand radicals	

### Applications/Properties

Acidochromism	peri-interactions
Adsorption	PH sensing
Aggregation induced emission (AIE)	Phosphorescence
Autoluminescence	Photocatalytic properties
Batteries/Electrochemistry	Photochemical properties
Bond activation	Photochromic properties
C-H bond activation	Photodegradation activity
Carbon monoxide releasing molecules (CORMs)	Photoinduced isomerization
Catalyst	Photoinduced oxidation
Charge transfer	Photoinduced structural reorganization
Chemosensors	Photoluminescence (PL)
Chromophores, Organic dyes	Photolytic reactivity
CO <sub>2</sub> fixation/reduction	Photophysical properties
Colorimetric sensing	Photosensitization
Dye adsorption	Photostability

Electric switches	Photoswitchable magnetism
Electrocatalytic properties	Porosity
Electrochemical properties	Precursor
Electrochemiluminescence	Proton conducting materials
Electroluminescence	Proton-coupled electron transfer (PCET)
Electron transfer	Recognition of a small organic molecule
Energy transfer	Redox properties
Excimer formation	Redox-catalytic reactions
Fluorescence	Selective sensor for a metal ion
Fluorescence quenching	Selective sensor for anion
Fluorescent redox switches	Selective sensor for discrimination of isomers
Frustrated Lewis pairs (FLP)	Selective sensor for NAE (nitroaromatic explosives)
Gas adsorption, Gas storage	Selective sensor for organic solvents
Gas sensors	Sensor
Gas separation	Single component molecular conductors (SCMC)
Gas separation	Single-chain-magnet
Host-guest fluorescence quenching	Single-component molecular metal (s-c conductor)
Intersystem crossing (ISC)	Single-ion magnet (SIM)
Ion detection	Single-molecule magnets (SMM)
Ionic fluorophores	Solar energy conversion, photocatalysis
Liquid phase separation	Solvatochromism
Luminescence	Spin-crossover (SCO)
Luminescence quenching	Temperature-responsive switches
Luminescence sensing	Thermally activated delayed fluorescence (TADF)
Luminescent sensing	Thermochromic luminescence
Luminescent sensors	Thermoelectric applications
Magneto-structural correlations	Thin film CVD (chemical vapor deposition) precursor
N-H bond activation	Up-conversion
Nitrite reduction	Vapochromism
Organic semiconductors	

## Methods

APCI-MS	MAS spectra
Circular dichroism spectroscopy (CD)	Mass spectrometry

Cold spray ionization mass spectrometry (CSI-MS)	Photoelectron spectroscopy
Cyclovoltammetry (CV)	Photoluminescence (PL)
Electrospray ionization mass spectrometry (ESI-MS)	SEM image
HF-EPR	Size exclusion chromatography (SEC)
HPLC	Spectroelectrochemistry
Inelastic Neutron Scattering (INS)	TEM image
LED-NMR spectroscopy	UV/vis emission spectroscopy
Magnetic circular dichroism spectroscopy (MCD)	UV/vis-NIR Spectroelectrochemistry
MALDI-TOF mass spectrometry	

### Nuclearity

Binuclear complexes	Polynuclear complexes
Heterometallic complexes	Tetranuclear complexes
Mononuclear complexes	Trinuclear complexes
no metal atoms	

### Denticity

Bidentate ligand	Pentadentate ligand
Bridging ligand	Pincer ligand
Hexadentate ligand	Tetradentate ligand
Monodentate ligand	Tridentate ligand
Multidentate ligand	