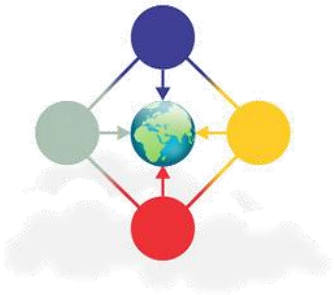
Materials Platform for Data Science(MPDS)のご紹介

Cliffhanger株式会社

Materials Platform for Data Science (MPDS) とは

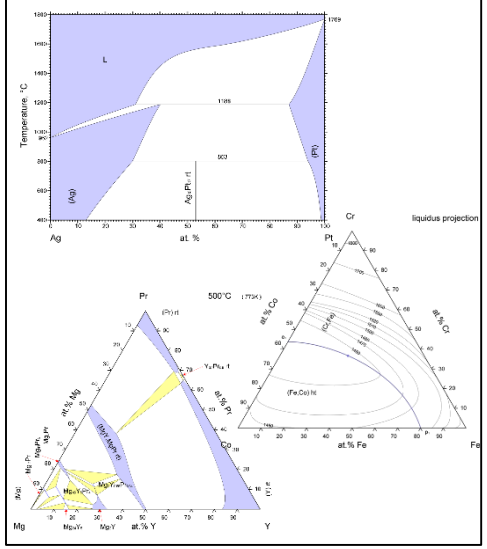


Materials Platform for Data Science(MPDS)は、材料の物性データを提供するデータベースです。
- Pauling Fileデータベースの30万件を超える査読付き論文情報
- 第一原理計算結果(MPDSオリジナル・7万件以上)
- 機械学習結果（MPDSオリジナル・90万件以上)

が登録されています。
全てのデータはブラウザベースのグラフィカルユーザーインターフェース(GUI)と
アプリケーションプログラミングインターフェース(API)の二つの方法で提供されています。

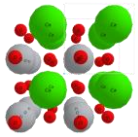
データベース

状態図



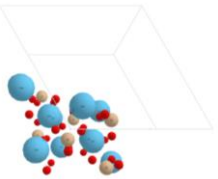
※ based on Pauling File

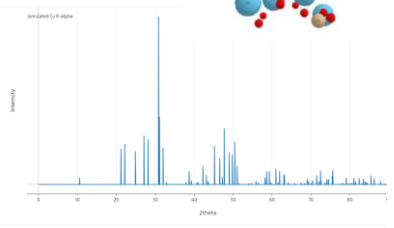
結晶構造



$CaTiO_3$

$La_{4.67}[SiO_4]_3O$





cifファイル、inputファイルをダウンロード可能

※ based on Pauling File

材料特性

- 光学特性
- 相転移
- 電気特性
- 超電導特性
- 磁気特性
- 機械特性
- 熱・熱機械的特性

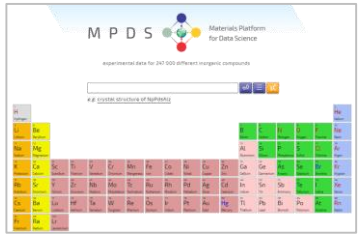
詳しくは次ページに記載

※ based on Pauling File
and MPDS inhouse data

プラットフォーム

GUIアクセス

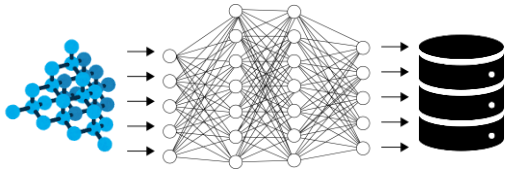
直感的な操作が可能
プログラミングの知識は
必要なし



APIアクセス

Pythonクライアント
(http)を提供

機械学習に最適



MPDSで取り扱われている材料物性

optical properties

optical conductivity	optical conductivity, real part of optical conductivity, imaginary part of optical conductivity
optical absorption coefficient	transmittance, optical absorption coefficient
plasma edge	plasma frequency, plasma edge
values of luminescence	luminescence lifetimes, wavelength for luminescence
phonons	energy of transverse optical phonon wavenumber of longitudinal optical phonon, wavenumber of optical phonon, wavenumber of transverse optical phonon, energy of longitudinal optical phonon, energy of optical phonon
work function	work function
refractive index	extraordinary refractive index, pressure dependence of refractive index, birefringence, refractive index, ordinary refractive index, temperature derivative of refractive index
reflectivity	reflectivity

superconductivity

values of superconductivity energy gap	values of superconductivity energy gap
critical magnetic field	critical magnetic field, upper critical magnetic field anisotropy, temperature derivative of upper critical magnetic field, lower critical magnetic field, temperature derivative of critical magnetic field, upper critical magnetic field, irreversibility field
superconducting transition temperature	superconducting transition temperature, composition derivative of superconducting transition, temperature, pressure derivative of superconducting transition temperature, lower superconducting transition temperature, lowest temperature of investigation, pressure dependence of superconducting transition temperature
critical current density	critical current density
coherence length	coherence length
electron-phonon interaction parameter	electron-phonon interaction parameter

mechanical properties

values of magnetostrictionc	spontaneous linear magnetostriction, saturation linear magnetostriction, spontaneous volume magnetostriction, volume magnetostriction, linear magnetostriction, magnetic field derivative of linear magnetostriction
values of sound velocity	values of sound velocity, transverse sound velocity, longitudinal sound velocity
values of elasticity	elastic compliance, temperature dependence of elastic stiffness coefficient, elastic stiffness coefficient, longitudinal-mode elastic coefficient, temperature derivative of elastic stiffness coefficient, elastic stiffness coefficient anisotropy, pressure derivative of elastic stiffness coefficient
values of elastic moduli	shear modulus, temperature derivative of isothermal bulk modulus, adiabatic bulk modulus, pressure derivative of isothermal bulk modulus, pressure derivative of adiabatic bulk modulus, isothermal bulk modulus, temperature derivative of adiabatic bulk modulus
ferroelasticity	paraelastic-ferroelastic transition temperature, spontaneous elastic strain
values of compressibility	isothermal linear compressibility, volume change at structural transition, mechanical cell parameters change, molar volume, adiabatic volume compressibility, isothermal volume, compressibility, volume change, pressure dependence of cell parameter
hardness	microhardness

electronic and electrical properties

electric field gradient	electric field gradient
values of conductivity or resistivity	ionic conductivity, temperature dependence of resistivity, pressure dependence of resistivity, electrical resistivity, electron conductivity, phonon resistivity, electrical conductivity, field dependence of resistivity, resistivity anisotropy, temperature derivative of resistivity, magnetic resistivity
electric polarization	electric polarization, electric dipole moment, spontaneous polarization
spin-fluctuation resistivity	spin-fluctuation resistivity
effective mass	effective mass of electrons, effective mass of polarons, effective mass of electrons to holes ratio, effective mass of electrons anisotropy
values of charge carrier concentration	donor concentration, effective electron number, electron to hole concentration ratio, values of charge carrier concentration, acceptor to donor concentration
values of ferroelectric hysteresis	remanent polarization, coercive electric field
pyroelectricity	pyroelectric coefficients
values of valence or charge transfer	average number of 3d electrons, valence electron concentration, average number of 4f electrons, effective charge, average number of 5f electrons
values of activation energy	acceptor energy, pressure derivative of activation energy, activation energy for migration of vacancies, values of activation energy, donor energy
metal or nonmetal character	temperature for metal-nonmetal transition, pressure for metal-nonmetal transition
permittivity dielectric constant	static permittivity, imaginary part of permittivity, pressure dependence of static permittivity, dielectric loss tangent, real part of permittivity, magnetic field dependence of permittivity, temperature dependence of static permittivity, high-frequency permittivity, volume strain dependence of high-frequency permittivity, volume strain dependence of static permittivity
values of charge carrier mobility	electron mobility, hole mobility, values of charge carrier mobility, electron to hole mobility ratio
values of residual resistivity	values of residual resistivity
piezoelectricity	piezoelectric coefficient
ferroelectric transitions	freezing temperature for relaxor, temperature for ferroelectric reordering
electronic energy gap	pressure derivative of energy gap for direct transition, pressure dependence of energy gap, thermal energy gap, charge-transfer energy, temperature derivative of energy gap for direct transition, exciton energy, temperature derivative of energy gap, pressure derivative of energy gap for indirect transition, volume strain dependence of energy gap for direct transition, energy gap for direct transition, pressure derivative of energy gap, electronic energy gap, energy gap for indirect transition, spin-orbit splitting of valence band, polaron formation energy

phase transition

eutectoid decomposition	temperature for eutectoid decomposition
fusion	temperature for congruent melting
values of peritectic formation	temperature for peritectic formation
decomposition	decomposition temperature
peritectoid formation	temperature for peritectoid formation
structural transition	temperature for structural transition, pressure derivative of transition temperature, pressure for structural transition, magnetic field for structural transition, composition derivative of transition temperature

magnetic properties

crystal electric field	crystal electric field splitting, crystal electric field, crystal field level
exchange field	exchange field, exchange interaction parameter
magnetic transitions	magnetic field for magnetic transition, freezing temperature for spin glass, pressure for magnetic transition, pressure derivative of temperature for magnetic transition, temperature for magnetic transition
spin-fluctuation	spin-fluctuation temperature
curie-weiss paramagnetism	molecular field parameter, paramagnetic moment, molecular field parameter
n tin orbital tb lmto method	spontaneous magnetic moment
values of magnetic susceptibility	paramagnetic contribution to magnetic susceptibility, temperature-independent, part of magnetic susceptibility, real part of magnetic permeability, valence-electron contribution to magnetic susceptibility, spin contribution to magnetic susceptibility, imaginary part of magnetic susceptibility, values of magnetic susceptibility, imaginary part of magnetic permeability, diamagnetic contribution to magnetic susceptibility, real part of magnetic susceptibility, magnetic permeability, pressure dependence of magnetic susceptibility, core-electron contribution to magnetic susceptibility, temperature derivative of magnetic susceptibility
magnetization	pressure dependence of saturation magnetic moment, saturation magnetic moment, magnetic moment, orbital magnetic moment, spontaneous magnetization, spin magnetic moment, magnetization, saturation magnetization
moessbauer spectra	isomer shift, quadrupole splitting, hyperfine magnetic field
values of magnetic anisotropy	second-order magnetocrystalline anisotropy coefficient, magnetic anisotropy energy, first-order magnetocrystalline anisotropy coefficient,magnetic anisotropy field
resonance spectra	quadrupole frequency
magnetic hysteresis	remanent magnetization, coercive field, remanent magnetic field energy product, remanent magnetic moment

thermal and thermodynamic properties

entropy	entropy of formation, magnetic entropy, entropy, entropy of reaction
values of thermoelectric power	seebeck coefficient, power factor, temperature derivative of thermoelectric power, thermoelectric figure of merit, relative cooling power
thermal expansion	volume thermal expansion coefficient, thermal strain, cell volume change, volume thermal expansion coefficient change. thermal cell parameters change, linear thermal expansion coefficient, temperature derivative of cell parameter
values of volume change at phase transition	volume change at melting point, cell parameter change at phase transition, cell volume change at phase transition, length change at phase transition, values of volume change at phase transition
values of entropy change at phase transition	entropy change at melting point, values of entropy change at phase transition
heat capacity	coefficient of third-order term in heat capacity, electronic heat capacity coefficient, coefficient of fifth-order term in heat capacity, electronic contribution to superconducting heat capacity, magnetic heat capacity, adiabatic temperature change, phonon heat capacity at constant pressure, heat capacity at constant volume, heat capacity at constant pressure, electronic contribution to heat capacity, superconducting heat capacity
enthalpy or energy	enthalpy of reaction, enthalpy change, enthalpy of formation
values of thermal conductivity	values of thermal conductivity, phonon contribution to thermal conductivity, electronic contribution to thermal conductivity
heat capacity discontinuity	heat capacity discontinuity at superconducting transition, heat capacity discontinuity, heat capacity discontinuity at structural transition
enthalpy change at phase transition	enthalpy change at melting point, enthalpy change at structural transition, enthalpy change at eutectoid decomposition, enthalpy change at decomposition. enthalpy of sublimation

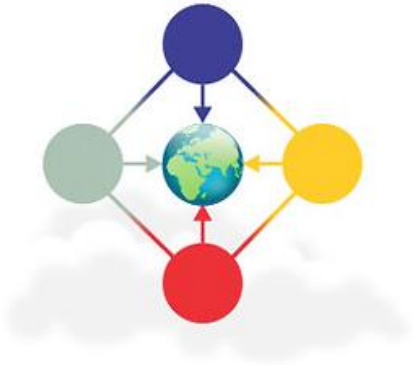
MPDSをご利用の企業様

Sumsung、上海大学を始め、多くの企業がMPDSを導入をしています。

主な大規模材料物性データベース

	実験系	シミュレーション系（第一原理計算）
基礎的	• MPDS • AtomWork (NIMS提供・有償版と無償版がある) • ICSD (日本では科学情報協会提供)	• The Materials Project (https://next-gen.materialsproject.org/)
実用的	• MatWeb (https://www.matweb.com/) • Total Materia (https://www.totalmateria.com/ja/)	

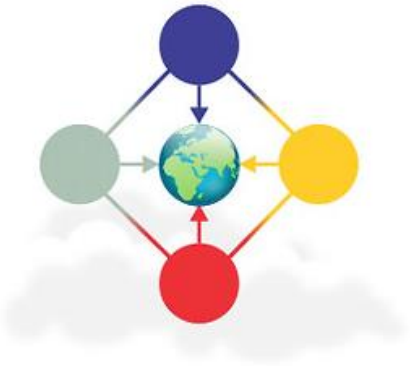
MPDSの料金体系



MPDS オープンアクセスカウント
¥0
MPDSのGUIとAPIの一部を
利用可能です。

導入前のトライアルにご利用ください

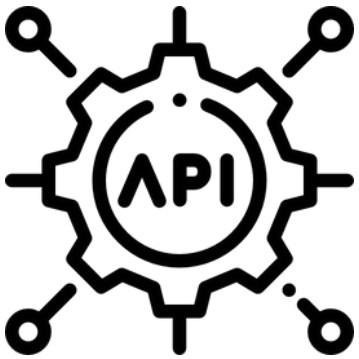
https://mpds.io/
メールアドレスの登録で利用可能です。
GitHub、ORCID、LinkedInの
アカウントでも利用できます。



MPDS GUIアカウント
¥360,000 (税別）
MPDSのGUIを使用する権利となります。
APIも一部利用可能です。

長期で契約すればするほど、
お得になります

1年契約: 1年あたり360,000円 (税別)
2年契約: 1年あたり340,000円 (税別)
3年契約: 1年あたり320,000円 (税別)



MPDS APIアカウント
¥1,500,000 (税別)
MPDSのGUI及びAPIを使用する
権利となります。

長期で契約すればするほど、
お得になります

1年契約: 1年あたり1,500,000円 (税別)
2年契約: 1年あたり1,480,000円 (税別)
3年契約: 1年あたり1,460,000円 (税別)

※2024年9月3日 価格改定