专业助力创新

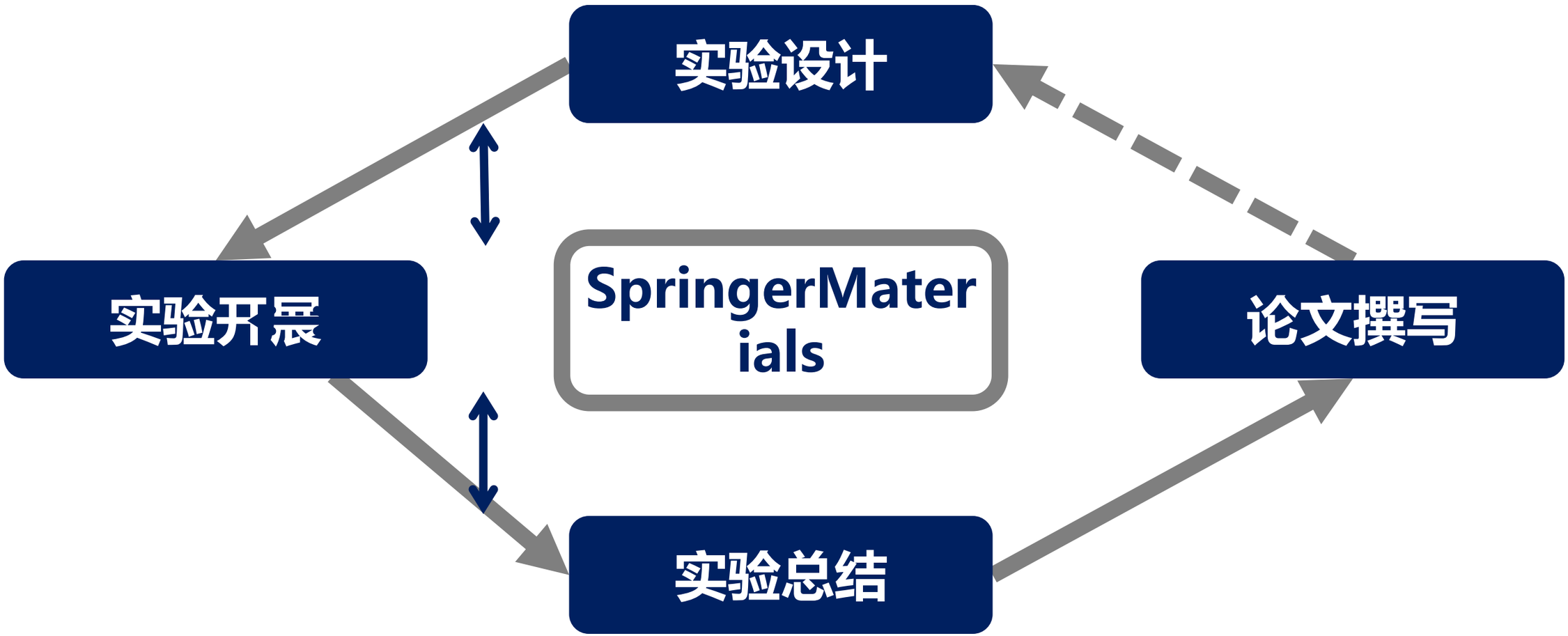
SpringerMaterials数据库的应用体会

Springer

中国科学技术大学图书馆

樊亚芳

文献调研是科研创新的基础



SpringerMaterials数据库简介

- SpringerMaterials数据库以Landolt-Börnstein科学与技术数值数据和函数关系丛书（简称LB丛书）为基础，是最大的材料学及物理和化学数据资源，是一个独特的高质量数值型数据库，内容涵盖了精选的、经过严格评估的材料物理化学和工程科学的各个领域的数据。这些数据使科学家们可以快速访问物质特性、函数关系以及数值数据，从而节省了宝贵的科研时间

SpringerMaterials数据库的主要功能

- 多种检索途径（快速、元素周期表和结构检索）
- 经过深度加工的数据整合
- 按性质聚类和精炼检索结果
- 提供用于原始数据筛选的滑动条
- 拥有精确坐标的相图
- 三维交互式结构

多种检索途径

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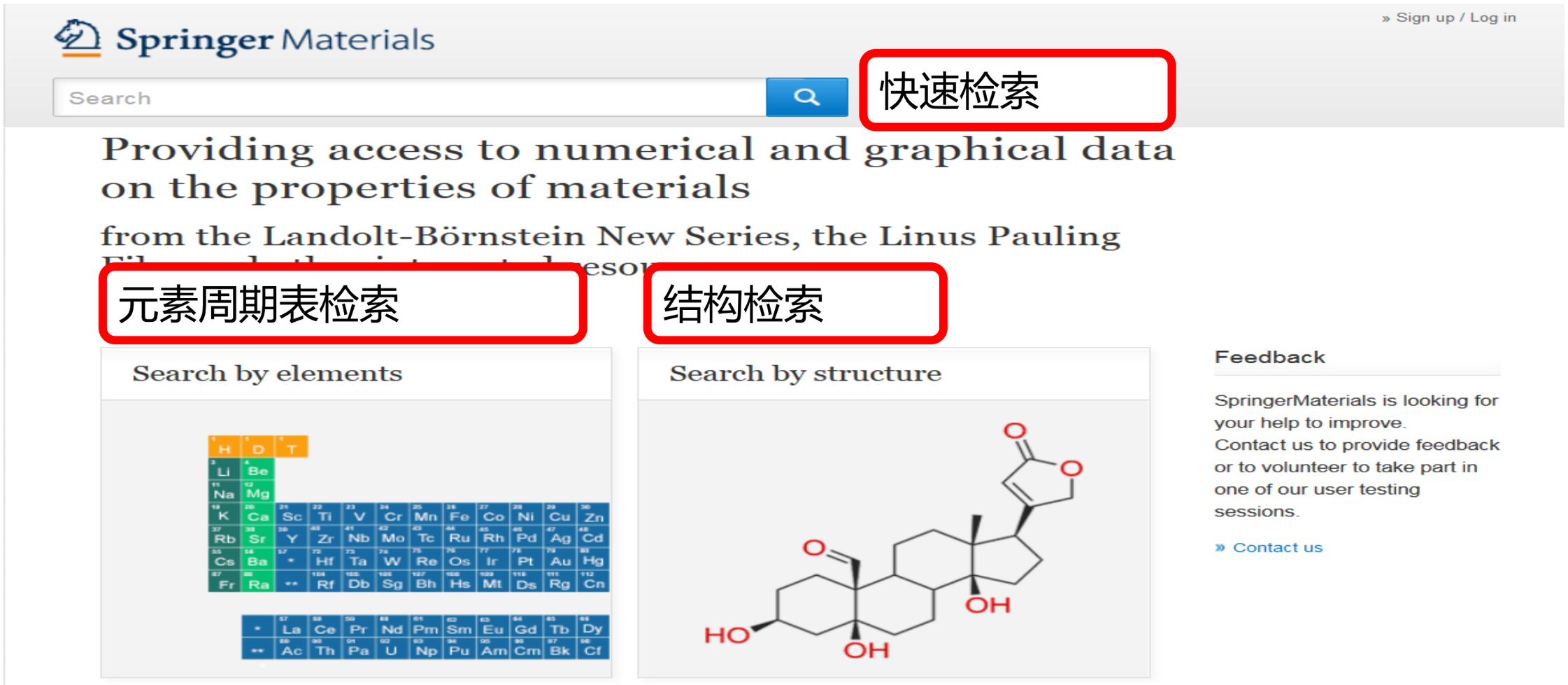

快速检索（graphene）

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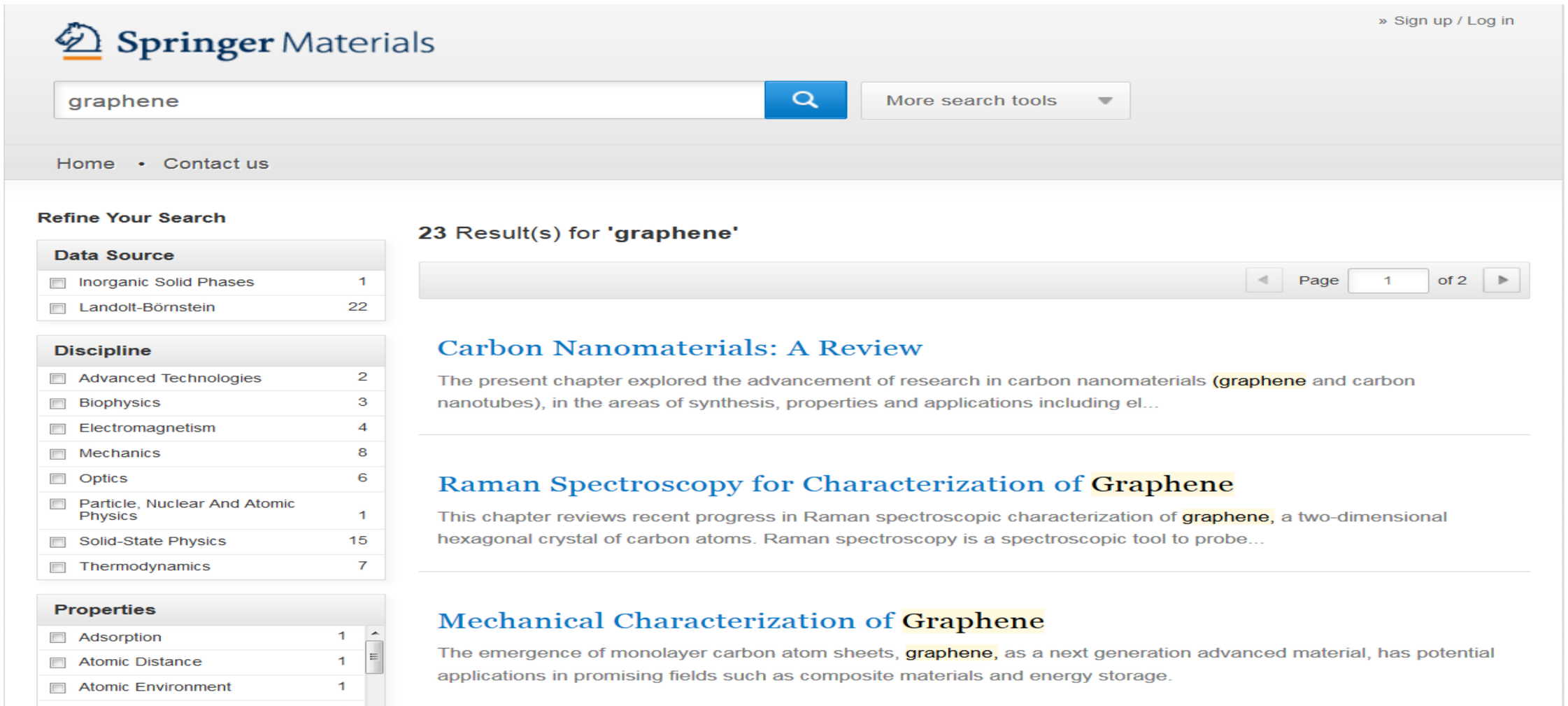

关于石墨烯的综述

Springer

Carbon Nanomaterials: A Review

Abstract

The present chapter explored the advancement of research in carbon nanomaterials (graphene and carbon nanotubes), in the areas of synthesis, properties and applications including electronics, field emission, biological and energy applications. The reported properties and applications of these carbon nanomaterials have opened up new opportunities for the future devices and materials. The knowledge presented here should lead to a better understanding of the key factors that can influence the future research directions.

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References (354)

About the Content

Title
Carbon Nanomaterials: A Review

Book Title
Handbook of Nanomaterials Properties

Book DOI
10.1007/978-3-642-31107-9

Editors
Bharat Bhushan (1)
Dan Luo (2)
Scott R. Schricker (3)
Wolfgang Sigmund (4)
Stefan Zauscher (5)

Editor Affiliation
1 Nanoprobe Laboratory for Bio- & Nanotechnology and Biomimetics,

关于石墨烯的综述

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Bookmarks

- 21 Carbon Nanomaterials: A Review
  - Introduction
  - Properties of Carbon Nanomaterials
    - Properties of Carbon Nanotubes (CNTs)
      - Electrical Properties
      - Mechanical Properties
      - Thermal Properties
    - Properties of Graphene
      - Mechanical Properties of Graphene
      - Electrical Properties of Graphene
      - Thermal Properties of Graphene
  - Synthesis of Carbon Nanomaterials
    - Synthesis of CNT
      - Arc Discharge
      - Laser Ablation
      - Chemical Vapor Deposition
    - Synthesis of Graphene
      - Thermal CVD
      - PECVD
      - SiC Sublimation
      - Exfoliation
      - Others
  - Applications of Carbon Nanomaterials

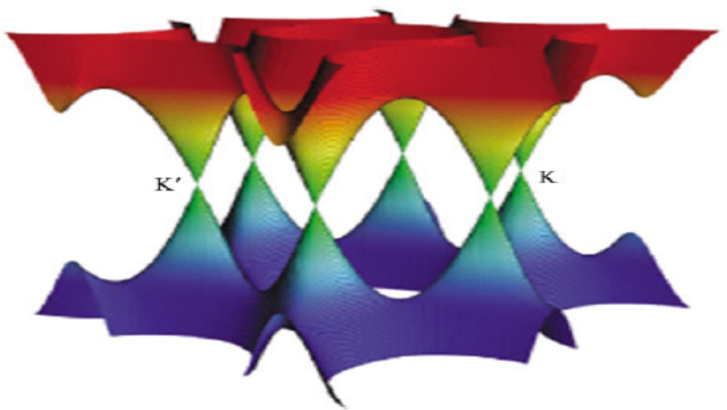

Fig. 21.11 Electronic band structure of single-layer graphene (Reprinted with permission from Katsnelson et al. [72]. Copyright (2007): Elsevier)

Electrical Properties of Graphene

One of the hottest areas of graphene research focuses on the intrinsic electronic properties as how electrons flow through a one-atom-thick sheet under the influence of various external forces [70, 71]. Graphene is great conductor, and thereby electrons are able to flow through graphene more easily than through even copper. The electrons travel through the graphene sheet as if they carry no mass, as fast as just one hundredth that of the speed of light. Single-layer graphene (SLG) is unique in electronic structure, as it shows band overlap in two conical points (K and K') in the Brillouin zone (Fig. 21.11) [72]. The charge carriers in this structure, known as massless Dirac fermions, are electrons losing their rest mass, m_o, and can best be described by (2 + 1)-dimensional Dirac equations. Thus, SLG is expected to show some unusual properties, as compared with metals and semiconductors and typical

石墨烯的拉曼光谱

Springer

Raman Spectroscopy for Characterization of Graphene

Abstract

This chapter reviews recent progress in Raman spectroscopic characterization of graphene, a two-dimensional hexagonal crystal of carbon atoms. Raman spectroscopy is a spectroscopic tool to probe scattering of light by phonons in graphene and used to study the structural and electronic properties. Crystal structure and band structure of graphene is explained. Raman spectra of graphene and graphite are shown. A typical confocal micro-Raman spectroscopy system is shown. Polarized Raman spectroscopy has proven to be a powerful tool in the study of the properties of graphene. Uniaxial strain breaks the in-plane isotropy and produces many interesting effects. The most important application of Raman spectroscopy in graphene research is to estimate the number of graphene layers. The interference effect can be quantitatively analyzed using a multireflection model (MRM) of the Raman scattered light. Controlling the charge carrier type and density is a key to electronic device application of graphene. Unlike most solids, graphene has a negative thermal expansion coefficient near the room temperature. Uniaxial or biaxial strain applied to a sheet of graphene alters the interatomic distance and modifies the crystal structure, two of the fundamental parameters that determine the properties of graphene. Since an edge of a graphene sample is a kind of a line defect, it induces defect mediated Raman scattering. Raman spectroscopy has proven to be an invaluable tool in graphene research owing to the unique features of graphene's physical properties.

References (59)

石墨烯的拉曼光谱

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Bookmarks

- 9 Raman Spectroscopy for Characterization of Graphene
  - 1 Definition of the Topic
  - 2 Overview
  - 3 Introduction
    - 3.1 Graphene
    - 3.2 Crystal Structure
    - 3.3 Band Structure
    - 3.4 Raman Scattering in Graphene
  - 4 Experimental and Instrumental Methodology
    - 4.1 Micro-Raman Spectroscopy
    - 4.2 Polarization
    - 4.3 Strain
  - 5 Key Research Findings
    - 5.1 Determination of Number of Graphene Layers
    - 5.2 Interference Effect
    - 5.3 Effect of Charge Carriers
    - 5.4 Thermal Effect
    - 5.5 Strain Effect
    - 5.6 Edges
    - 5.7 Stacking
  - 6 Conclusions and Future Perspective
  - References

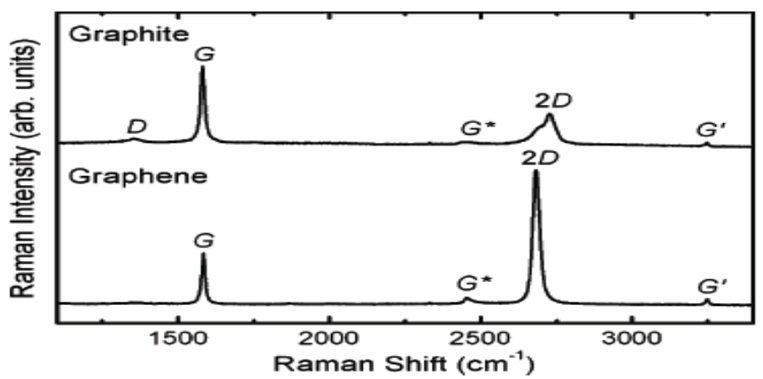

Fig. 9.6 Raman spectra of graphene and graphite

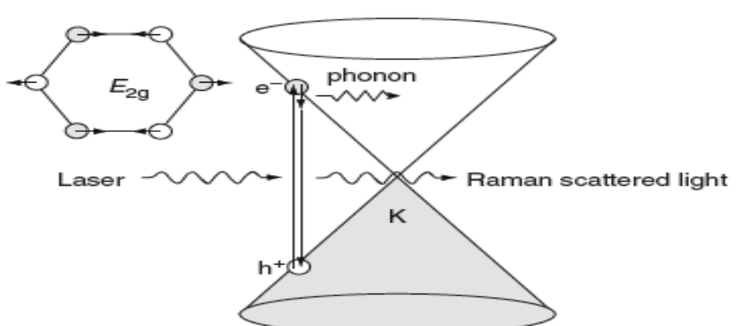

Fig. 9.7 Vibration of E_{2g} phonon mode and the resonant Raman scattering process for the G band

快速检索（TiO_2）

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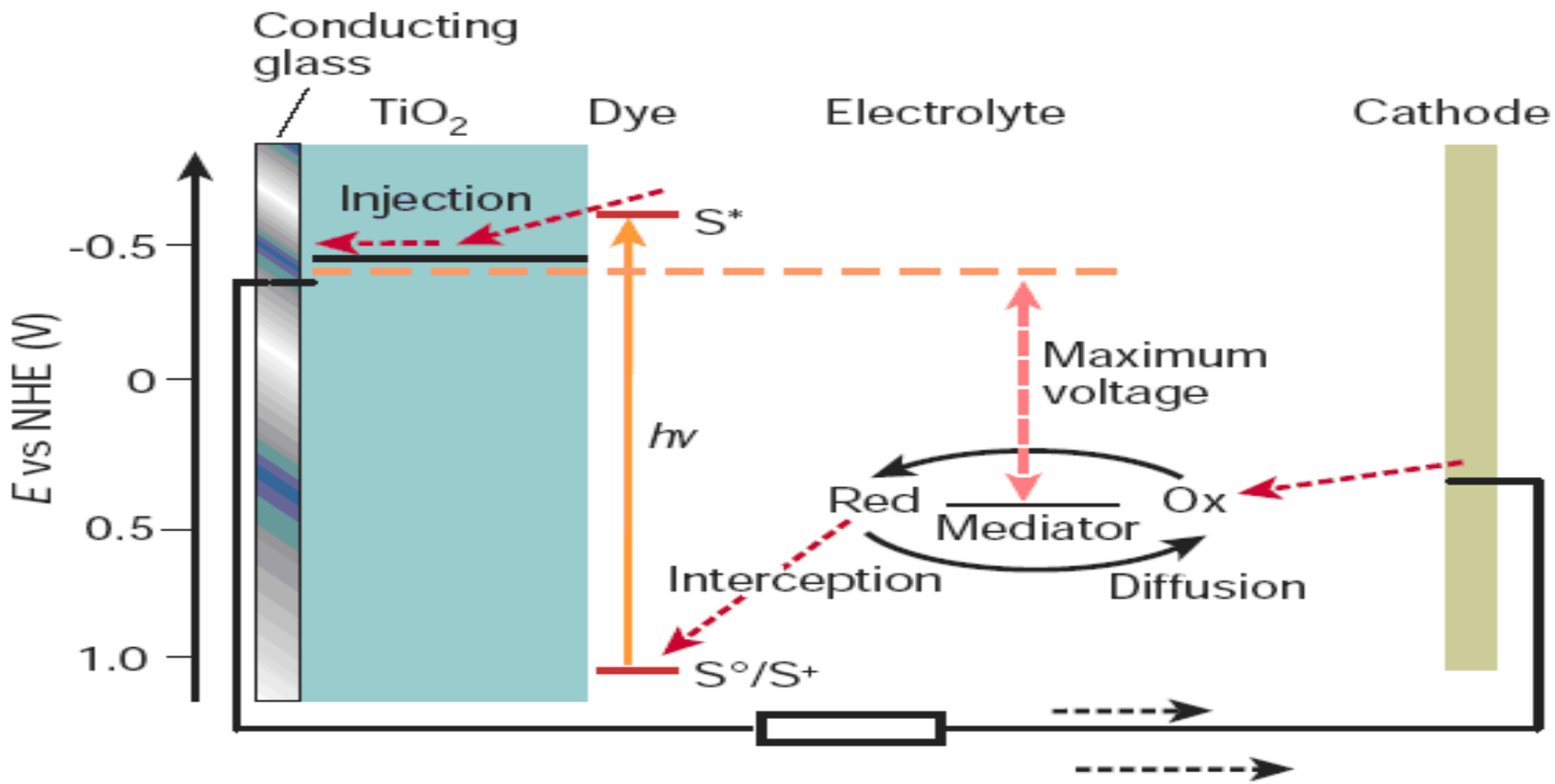
◆染料敏化太阳能电池中TiO_2的电子传递性能



WOS平台检索结果

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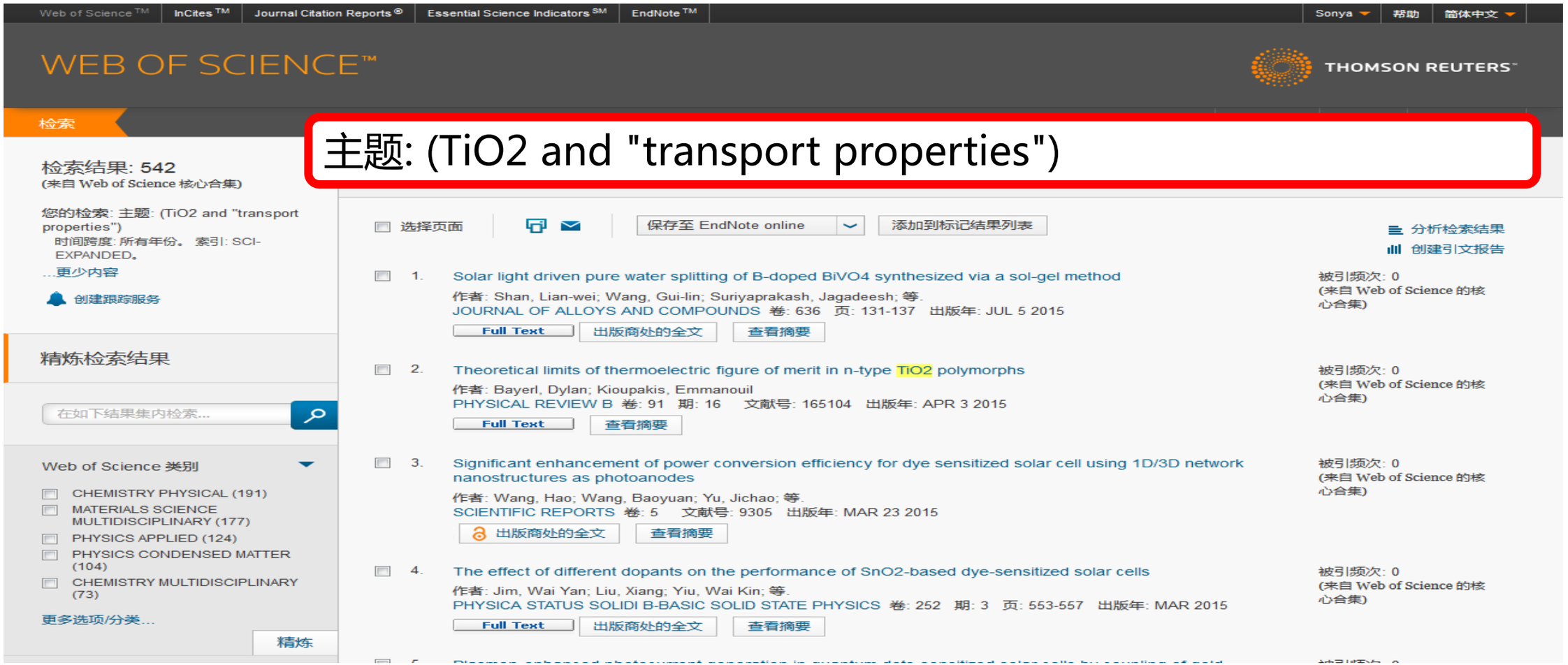
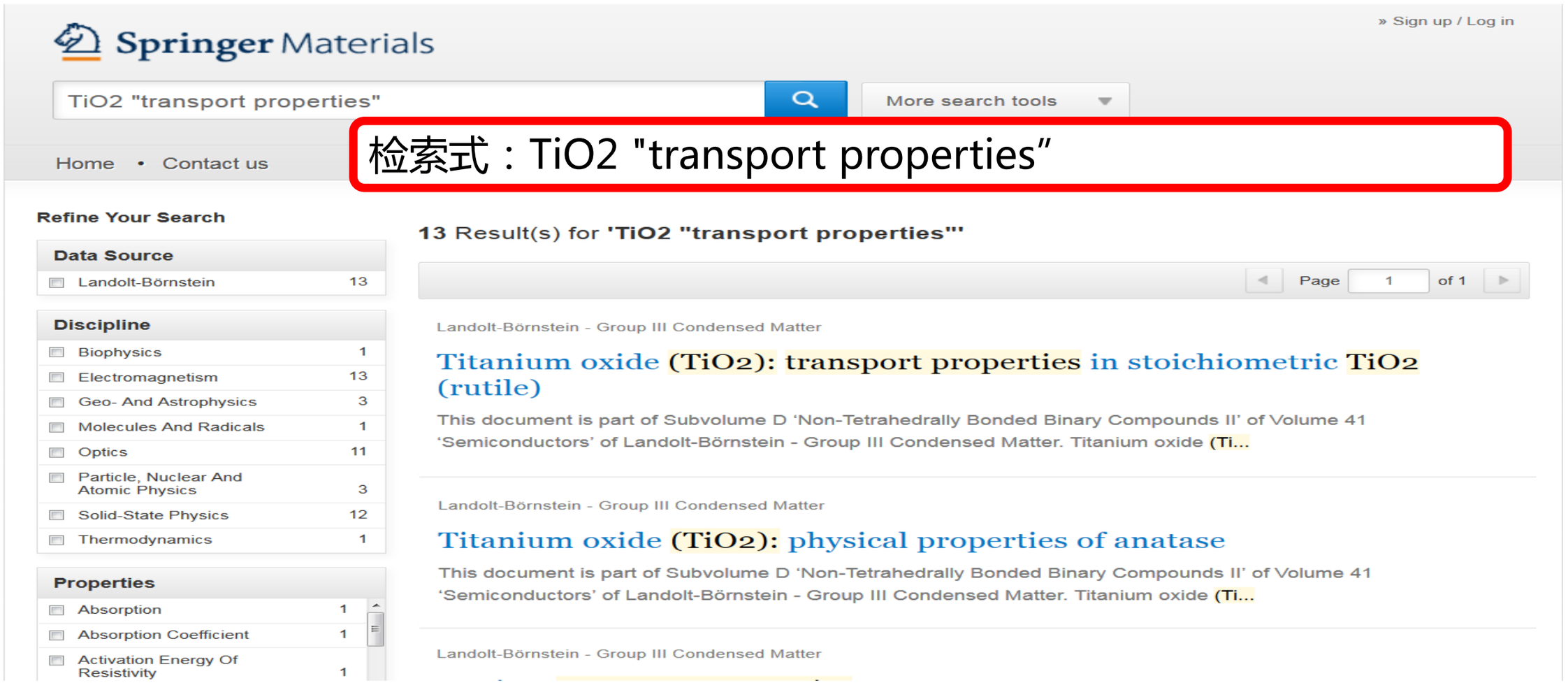


快速检索（TiO_2）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TiO2 "transport properties"
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检索式：TiO2 "transport properties”
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Landolt-Börnstein 13
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Biophysics 1
Electromagnetism 13
Geo- And Astrophysics 3
Molecules And Radicals 1
Optics 11
Particle, Nuclear And Atomic Physics 3
Solid-State Physics 12
Thermodynamics 1
Properties
Absorption 1
Absorption Coefficient 1
Activation Energy Of Resistivity 1
13 Result(s) for 'TiO2 "transport properties"'
Page 1 of 1
Landolt-Börnstein - Group III Condensed Matter
Titanium oxide (TiO2): transport properties in stoichiometric TiO2 (rutile)
This document is part of Subvolume D 'Non-Tetrahedrally Bonded Binary Compounds II' of Volume 41 'Semiconductors' of Landolt-Börnstein - Group III Condensed Matter. Titanium oxide (Ti...
Landolt-Börnstein - Group III Condensed Matter
Titanium oxide (TiO2): physical properties of anatase
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锐钛矿型TiO_2的电子传递情况

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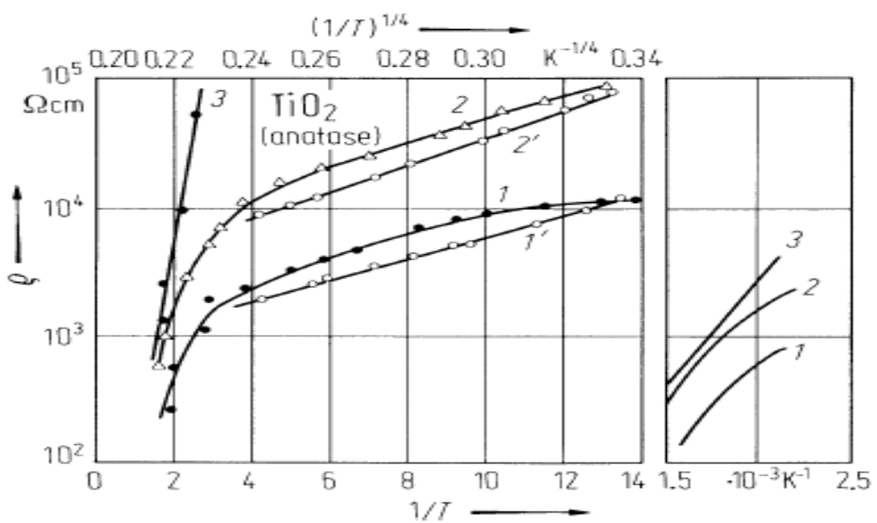
substance: titanium oxide (TiO_2)
property: physical properties of anatase
energy gap

Fig. 5.

TiO_2. Electrical resistivity of anatase modification vs. temperature. Curves *1...3*: ρ vs. $10^3/T$ for three (unoriented) samples of differing dopant level; curves *1'*, *2'*: ρ vs. $(1/T)^{1/4}$ for the two (unoriented) samples of lower resistivity [78V].



元素周期表检索（Al-O）

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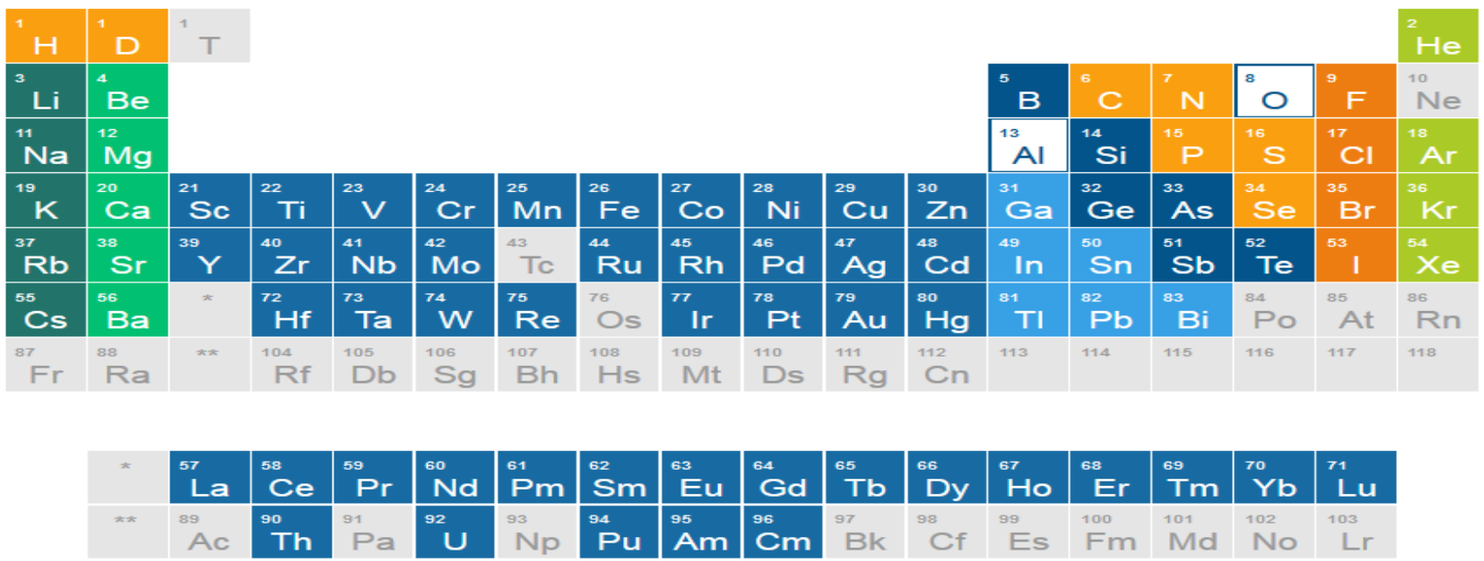
Search for information by element system



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Your Selection
Al-O

3504 Matching element systems

- Al-O (232)
- Ag-Al-O (31)
- Al-Am-O (2)
- Al-Ar-O (1)
- Al-As-O (16)
- Al-Au-O (3)
- Al-B-O (27)
- Al-Ba-O (51)
- Al-Be-O (20)
- Al-Bi-O (14)
- Al-Br-O (3)
- Al-C-O (24)

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元素周期表检索（Al-O）

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Refine Your Search

Data Source

Inorganic Solid Phases	168
Landolt-Börnstein	61
MSI Eureka	3

Discipline

Advanced Technologies	153
Biophysics	155
Electromagnetism	168
Geo- And Astrophysics	8
Mechanics	17
Molecules And Radicals	23
Optics	10
Particle, Nuclear And Atomic Physics	72
Solid-State Physics	181
Thermodynamics	25

Properties

Absorption	1
Absorption Coefficient	1
Activation Energy	1
Activity	1
Adsorbate Coverage	1
Adsorption	1
Asymmetry Parameter	2
Atomic Defect Properties	1
Atomic Environment	130

232 Result(s) for **'Al-O'**

◄ Page 1 of 12 ►

MSI Eureka © 2013 Report ID: 20.17148.1.1

Al-O Binary Phase Diagram Evaluation

Phase diagrams, crystallographic and thermodynamic data

The Al-O system is a part of industrially important... Review of experimental data for the Al-O system is presented in [

MSI Eureka

Phase diagram of the Al-O system

Temperature: 427...3727 °C

Concentration Range: Al conc. [100-0 at.%] / O conc. [0-100 at.%]

Part of report on 'Al-O Binary Phase Diagram Evaluation'

MSI Eureka

Temperature - composition phase diagram of the Al-O system

Temperature: 427...3727 °C

Concentration Range: Al conc. [100-0 at.%] / O conc. [0-100 at.%]

Part of report on 'Al-Fe-O Ternary Phase Diagram Evaluation'

Landolt-Börnstein - Group III Condensed Matter

Al_2O_3 γ

This document is part of Subvolume A9 'Structure Types. Part 9: Space Groups (148) R-3 - (141) I41' of Volume 43 'Crystal Structures of Inorganic Compounds' of Landolt-Börnstein - Group III 'Condensed Matter'.

拥有精确坐标的交互式相图

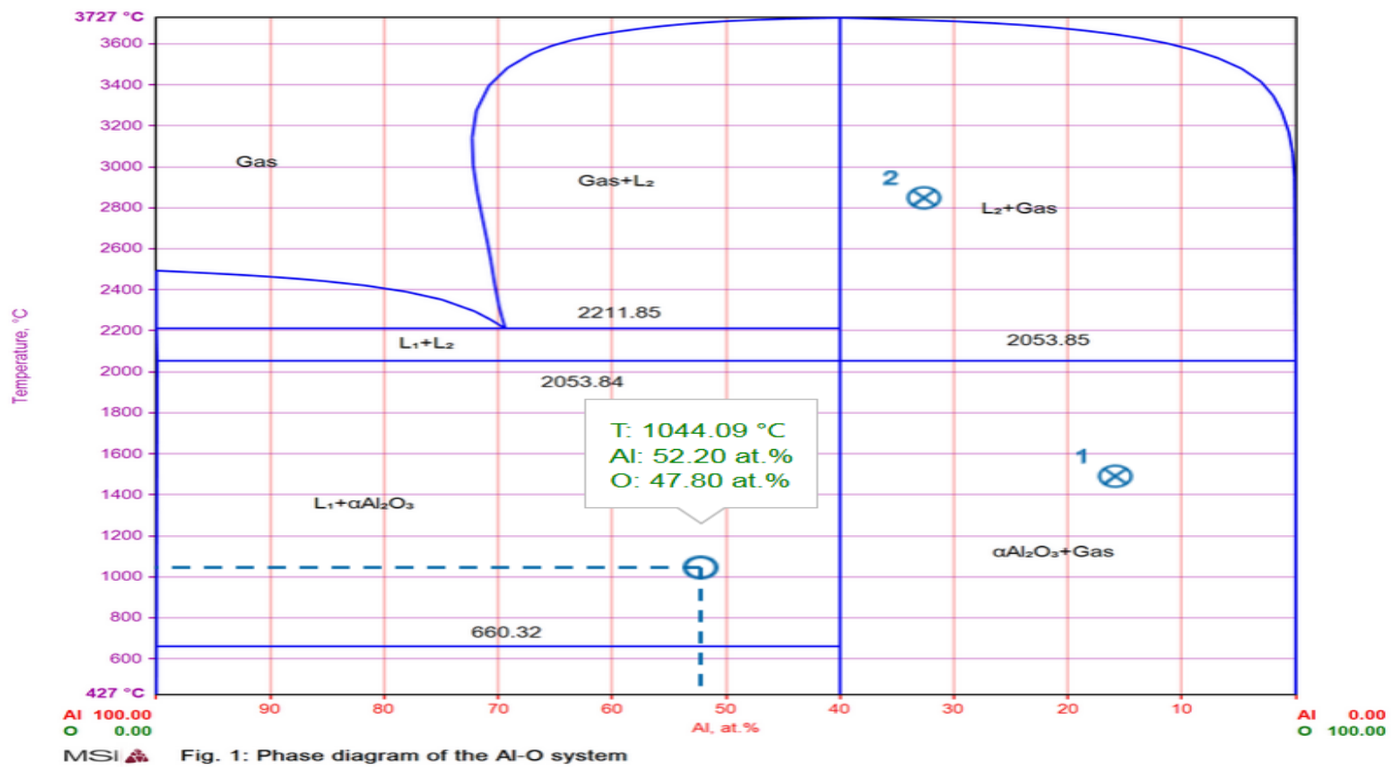


Fig. 1: Phase diagram of the Al-O system

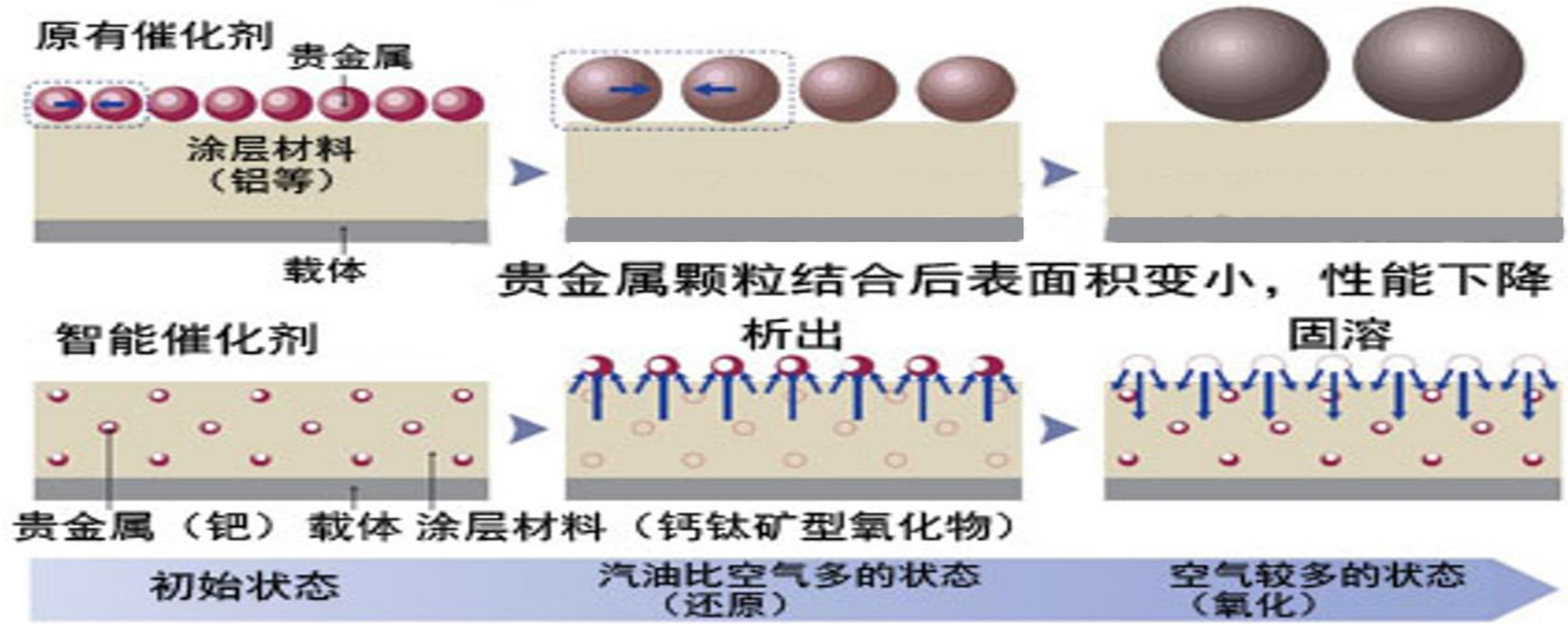
Recorded Points

Point 1
T: 1488.98 °C
Al: 15.84 at.%
O: 84.16 at.%

Point 2
T: 2845.88 °C
Al: 32.62 at.%
O: 67.38 at.%

元素周期表检索（$LaFePdO_3$）

◆用于汽车尾气净化的“智能催化剂”（$LaFePdO_3$）



元素周期表检索（$LaFePdO_3$）

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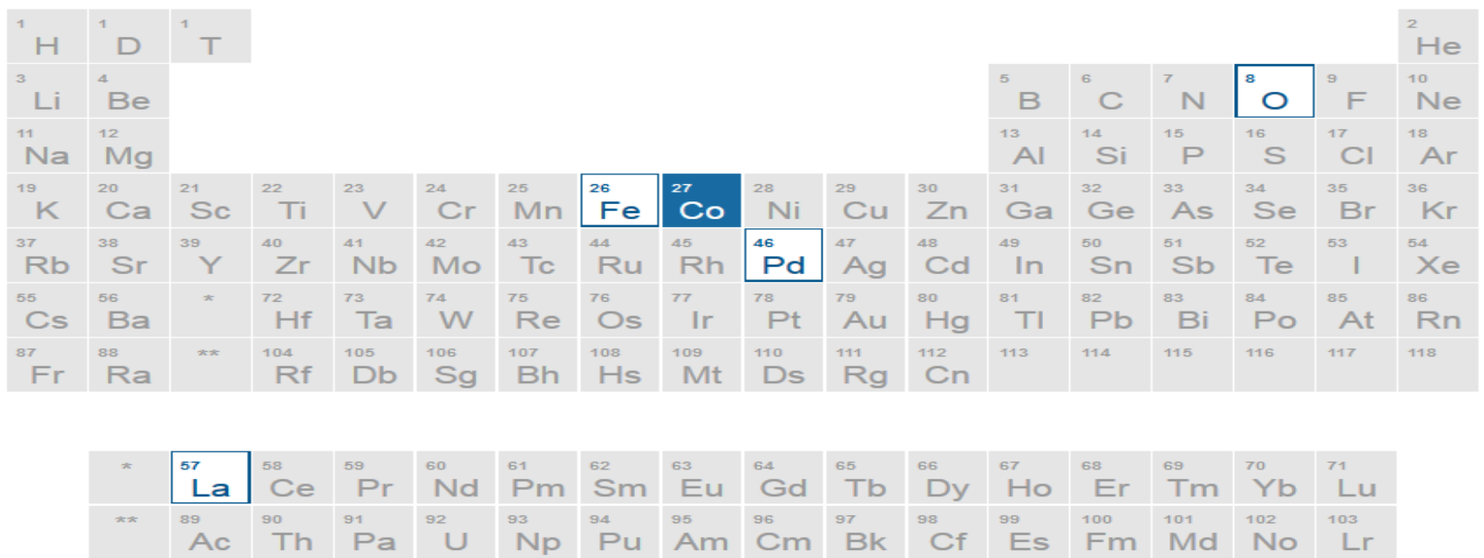
Search for information by element system



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Your Selection
Fe-La-O-Pd

2 Matching element systems

Fe-La-O-Pd (1)

Co-Fe-La-O-Pd (1)

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元素周期表检索（$LaFePdO_3$）

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Refine Your Search

Data Source

Inorganic Solid Phases	1

Discipline

Advanced Technologies	1
Biophysics	1
Electromagnetism	1
Solid-State Physics	1

Properties

Atomic Environment	1
Atomic Position	1
Cell Volume	1
Pearson Symbol	1
Positional Coordinate	1
Space Group	1
Unit Cell Axes	1
Unit Cell Parameter	1
Wyckoff Sequence	1
x-Ray Density	1

1 Result(s) for **'Fe-La-O-Pd'**

◄ Page 1 of 1 ►

Inorganic Solid Phases

$LaFe_{0.954}Pd_{0.046}O_3$ Crystal Structure

Element system Fe-La-O-Pd, Phase prototype $CaTiO_3$, Space group *cP*5, 221
Data on Cell parameters, Published and standardized atom coordinates

◄ Page 1 of 1 ►

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$LaFe_{0.954}Pd_{0.046}O_3$晶体结构

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Inorganic Solid Phases

$LaFe_{0.954}Pd_{0.046}O_3$ Crystal Structure

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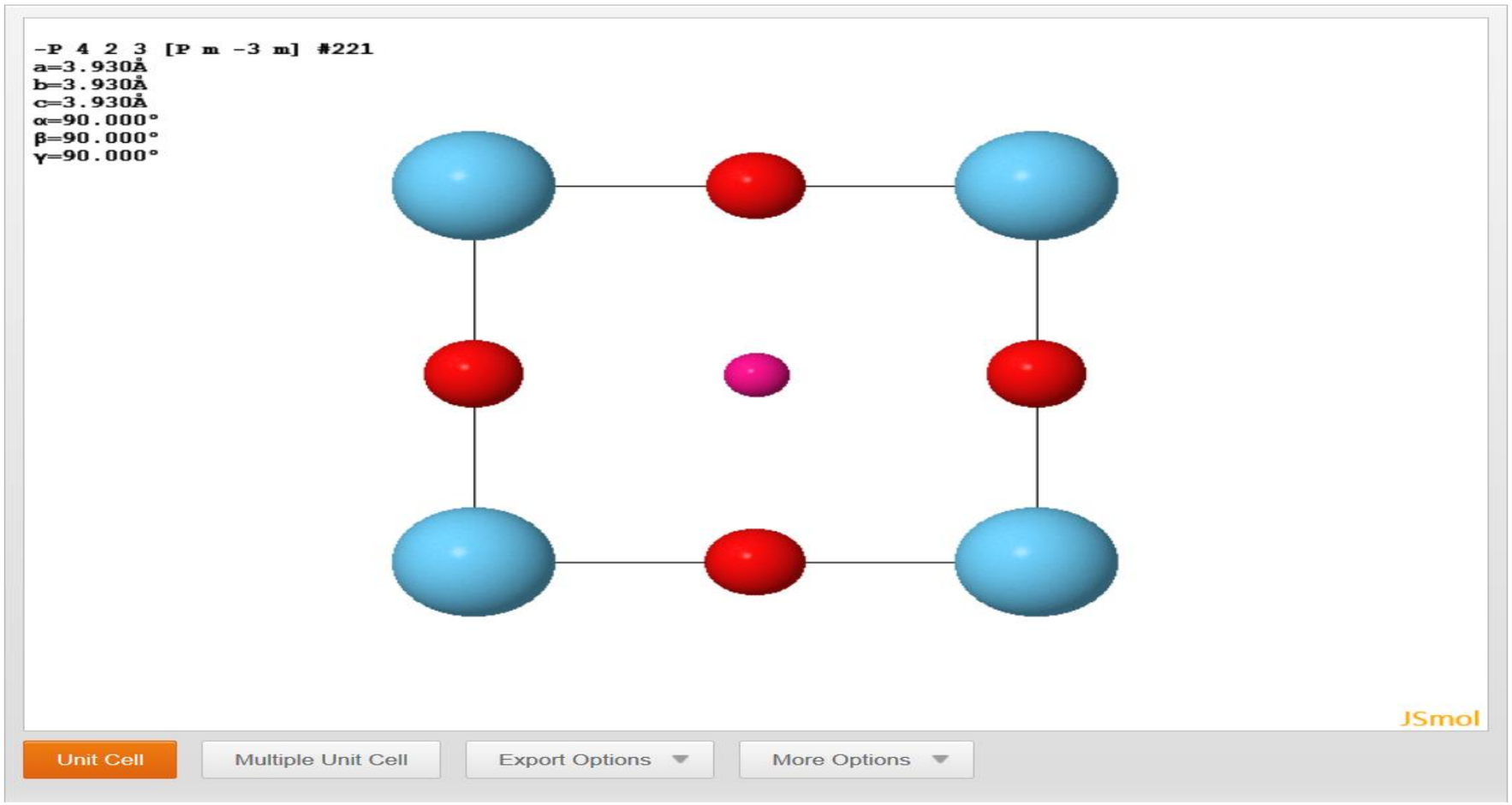
General Information

Phase Label(s): $LaFe_{0.954}Pd_{0.046}O_3$
Structure Class(es): perovskite
Classification by Properties: –
Mineral Name(s): –
Pearson Symbol: *cP*5
Space Group: 221
Phase Prototype: $CaTiO_3$
Measurement Detail(s): automatic diffractometer (determination of cell parameters), X-rays, Cu Kα (determination of cell parameters)
Phase Class(es): –
Compound Class(es): oxide
Interpretation Detail(s): cell parameters determined and type with fixed coordinates assigned
Sample Detail(s): sample prepared from La nitrate, Fe nitrate, $PdCl_2$, malic acid, atomic absorption spectroscopy; 2.0 wt.% Pd, powder (determination of cell parameters)

Substance Summary

Standard Formula: $LaFe_{0.954}Pd_{0.046}O_3$
Alphabetic Formula: $Fe_{0.954}LaO_3Pd_{0.046}$
Published Formula: $LaFe_{0.954}Pd_{0.046}O_3$
Refined Formula: $Fe_{0.95}LaO_3Pd_{0.05}$
Wyckoff Sequence: 221,dba

三维交互式结构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a=3.930Å
b=3.930Å
c=3.930Å
α=90.000°
β=90.000°
γ=90.000°
JSmol
Unit Cell
Multiple Unit Cell
Export Options
More Options

晶体学数据

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Crystallographic Data

Cell Parameters

Cell Parameters	Published Data	**Standardized Data**	
		Unit Cell	Niggli-Reduced Cell
Space Group	*Pm-3m* (221)	*Pm-3m* (221)	–
a	0.393 nm	0.393 nm	0.393 nm
b	0.393 nm	0.393 nm	0.393 nm
c	0.393 nm	0.393 nm	0.393 nm
α	90°	90°	90.°
β	90°	90°	90.°
γ	90°	90°	90.°
a/b	1.000	1.000	1.000
b/c	1.000	1.000	1.000
c/a	1.000	1.000	1.000

原子坐标

Atom Coordinates

Standardized

Site	Element	Wyckoff Symbol	Symmetry	X	Y	Z	Occupation	Co-Ord. No.	Atomic Env.
O	O	3*d*	4/mm.m	1/2	0	0	1	2	collinear, La_2
Fe,Pd	0.954Fe + 0.046Pd	1*b*	m-3m	1/2	1/2	1/2	1	12	cuboctahedron, O_{12}
La	La	1*a*	m-3m	0	0	0	1	6	octahedron, O_6

Transformation from Published to Standardized: No transformation from published to standardized cell parameters necessary.

Published

Site	Element	Wyckoff Symbol	Symmetry	X	Y	Z	Occupation
La	La	1*a*	m-3m	0	0	0	1
Fe,Pd	0.954Fe + 0.046Pd	1*b*	m-3m	1/2	1/2	1/2	1
O	O	3*d*	4/mm.m	1/2	0	0	1

实验细节

Experimental Details

Sample Details

analysis	atomic absorption spectroscopy; 2.0 wt.% Pd
samples	powder (determination of cell parameters)

Measurement Details

methods	automatic diffractometer (determination of cell parameters)
radiation	X-rays, Cu Kα (determination of cell parameters)

Interpretation Details

investigation	cell parameters determined and type with fixed coordinates assigned

Reference

Koponen M.J., Suvanto M., Pakkanen T.A., Kallinen K., Kinnunen T.J.J., Härkönen M.: *Syntheitic studies of ABB'O_3 (A= La, Pr, Nd; B= Fe, Mn; B'= Pd, Pt) perovskites*. Solid State Sciences **7** (2005) 7-12

元素周期表检索（Fe-La-O-Pd）

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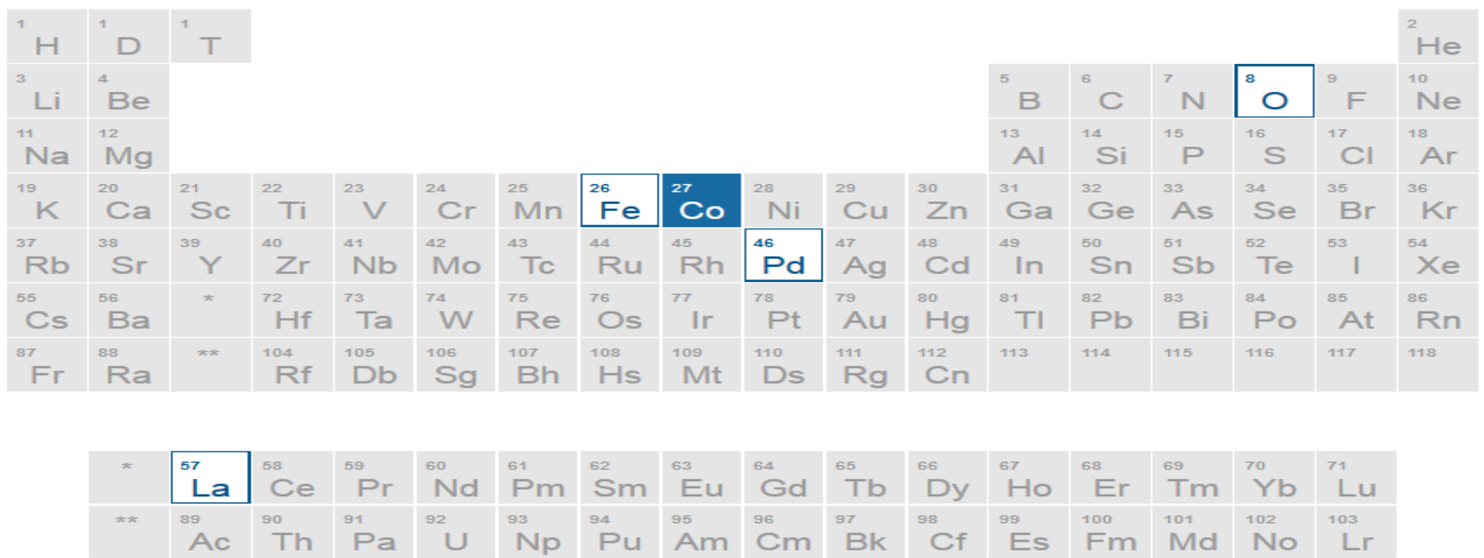
Search by Elements

Search for information by element system



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Your Selection
Fe-La-O-Pd

2 Matching element systems

Fe-La-O-Pd (1)

Co-Fe-La-O-Pd (1)

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$LaFe_{0.57}Co_{0.38}Pd_{0.05}O_3$晶体结构

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Inorganic Solid Phases

$LaFe_{0.57}Co_{0.38}Pd_{0.05}O_3$ Crystal Structure

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General Information

Phase Label(s): $LaFe_{0.57}Co_{0.38}Pd_{0.05}O_3$
Structure Class(es): perovskite
Classification by Properties: –
Mineral Name(s): –
Pearson Symbol: *cP5*
Space Group: 221
Phase Prototype: $CaTiO_3$
Measurement Detail(s): automatic diffractometer (determination of cell parameters), X-rays, Cu Kα (determination of cell parameters)
Phase Class(es): –
Compound Class(es): oxide
Interpretation Detail(s): cell parameters determined and type with fixed coordinates assigned

Reference

Koponen M.J., Suvanto M., Kallinen K., Kinnunen T.J.J., Härkönen M., Pakkanen T.A.: *Structural transformations in cubic structure of Mn/Co perovskites in reducing and oxidizing atmospheres*. Solid State Sciences **8** (2006) 450-456

结构检索：对二甲苯（PX）

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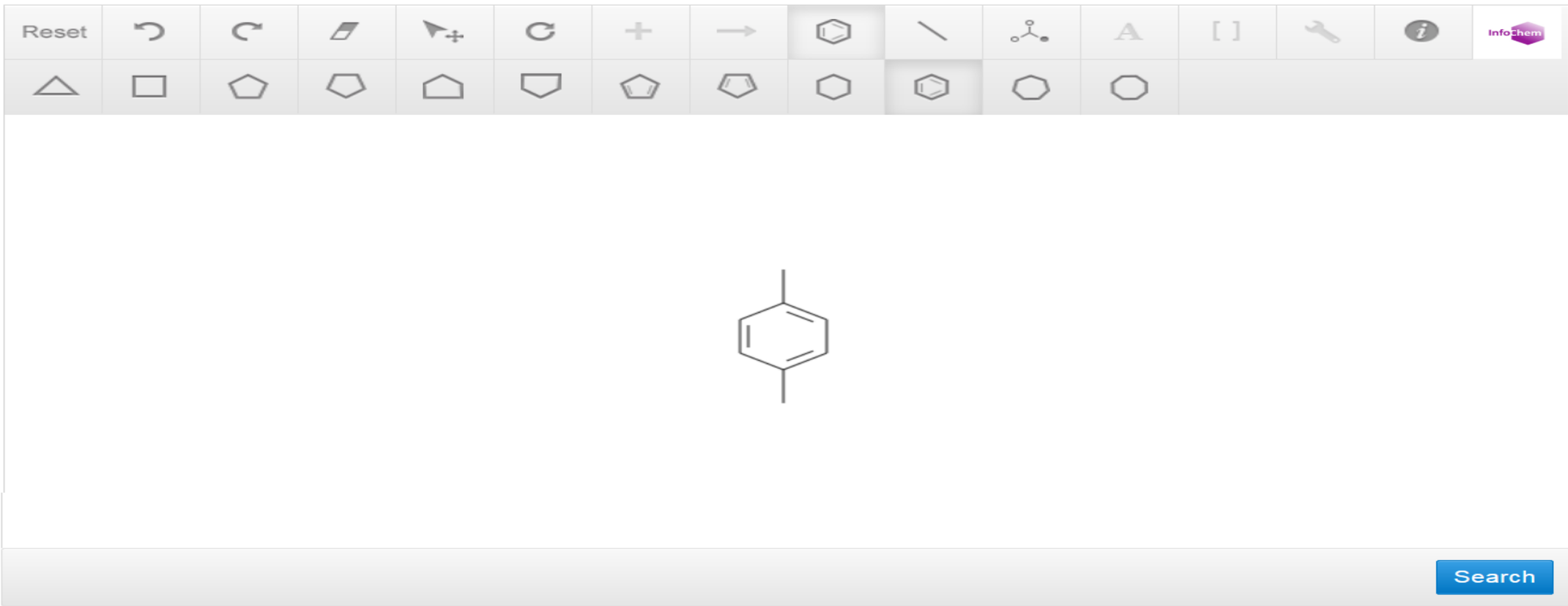
Search by Structure

Start by drawing a structure



结构检索结果（相似度排序）

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701 Result(s) for this structure

Page 1 of 36

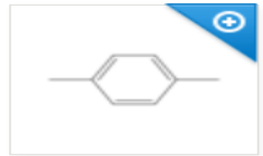
1,4-Dimethyl-Benzene

Molecular Formula: C_8H_{10}
Molecular Mass: -
CAS-No: 106-42-3

c1-7-3-5-8(2)6-4-7

VLBVBO-UHFFFAOYSA-N

» View substance profile » Search for this substance



100 % match

快速检索

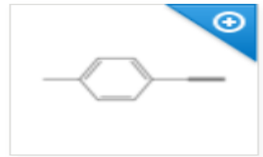
物质概况

-4-Methyl-

Molecular Formula: C_9H_8
Molecular Mass: -
CAS-No: 766-97-2

InchI: InChI=1S/C9H8/c1-3-9-6-4-8(2)5-7-9/h1,4-7H,2H3
InchI Key: KSZVOXHGCKKOLL-UHFFFAOYSA-N

» View substance profile » Search for this substance



91 % match

4-Methyl-Benzonitrile

Molecular Formula: C_8H_7N
Molecular Mass: -
CAS-No: 104-85-8

InchI: InChI=1S/C8H7N/c1-7-2-4-8(6-9)5-3-7/h2-5H,1H3
InchI Key: VCZNNAKNUVJVGX-UHFFFAOYSA-N

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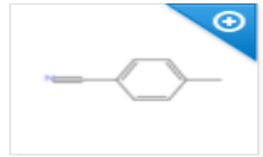

90 % match

物质概况

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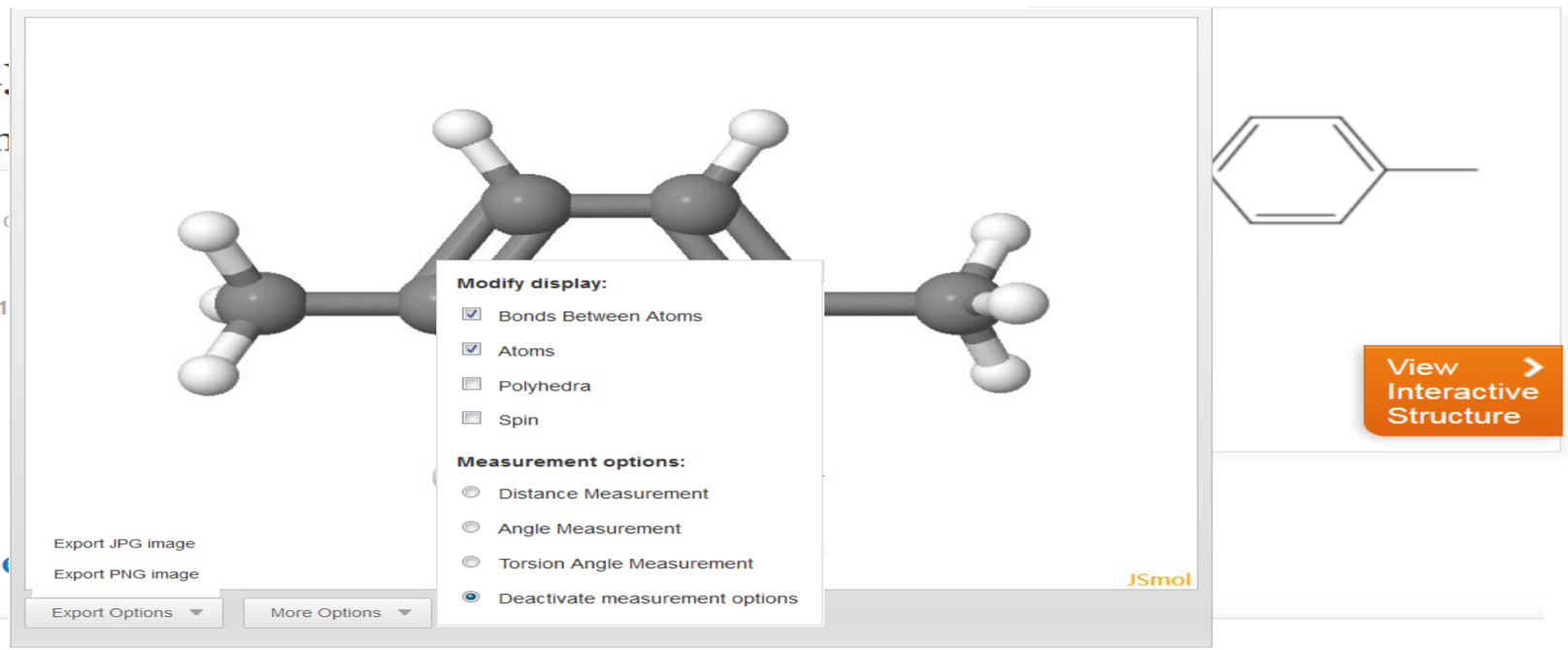
Substance Profile

1,4-Dimeth

General inforn

Molecular Formula: C_8H_{10}
Element System: C-H
CAS-RN: 106-42-3
InChI: InChI=1S/C8H10/c1



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3D Interactive

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Properties frequently appearing with 1,4-dimethyl-benzene

- » Osmotic Pressure (167)
- » Vapor-Liquid Equilibrium (151)
- » Excess Volume (99)
- » Heat Of Mixing (91)
- » Excess Enthalpy (91)
- » Polarization Degree (9)
- » Luminescence Emission Linewidth (9)
- » Luminescence (9)
- » Diffusion (8)
- » Chemical Diffusion (8)
- » Angular Frequency (1)
- » Transition Enthalpy (1)
- » Internuclear Distance (1)
- » Differential Scanning Calorimetry (1)
- » Phase Transition Temperature (1)

提供用于数据筛选的滑动条

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Vapor Pressure of p-Xylene

Filter data by:

Temperature [K] :

286.44 — 618.15

Hide Filter Tools

Temperature *T* [K]	Vapor Pressure *p* [kPa]	State	Reference
286.44	0.582	Vapor-Liquid	16. Osborn (1974)
288.15	0.649	Vapor-Liquid	16. Osborn (1974)
290.62	0.755	Vapor-Liquid	16. Osborn (1974)

References (102)

1. Panchenkov G.M., Maksareva T.S., Erchenkov V.V.: Temperature Dependence of Diffusion Coefficients of Some Organic Liquids. Zh.Fiz.Khim. 32 (1958) 2787-2791

2. Ambrose D., Broderick B.E., Townsend R.: The vapour pressures above the normal boiling point and the critical pressures of some aromatic hydrocarbons. J.Chem.Soc.A (1967) 633-641

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1,4-dimethyl-benzene

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Acentric Factor	1

701 Result(s)

Substance: 1,4-dimethyl-benzene

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Landolt-Börnstein - Group II Molecules and Radicals

Diamagnetic bulk susceptibility data of C_8H_{10}

This document is part of Subvolume B 'Diamagnetic Susceptibility of Organic Compounds, Oils, Paraffins and Polyethylenes' of Volume 27 'Diamagnetic Susceptibility and Anisotropy' of Landolt-Börnstein - Group...

Landolt-Börnstein - Group IV Physical Chemistry

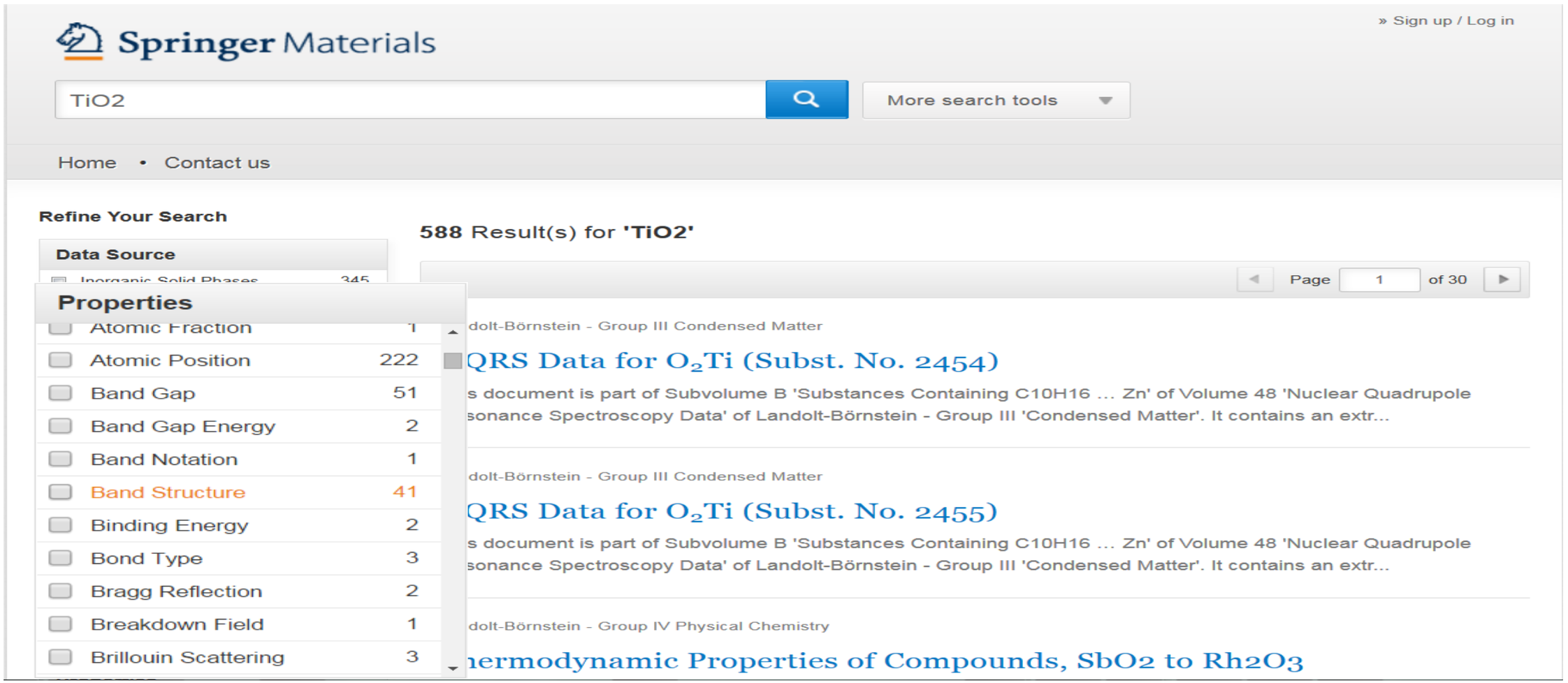
Dielectric constant of the mixture (1) 2-methoxyaniline; (2) 1,4-dimethylbenzene

This document is part of Volume 17 'Static Dielectric Constants of Pure Liquids and Binary Liquid Mixtures (Supplement to IV/6)' of Landolt-Börnstein Group IV 'Physical Chemistry'.

Thermophysical Properties

Tetrachloromethane-p-Xylene Excess Volume

按性质聚类和精炼检索结果



按性质聚类和精炼检索结果

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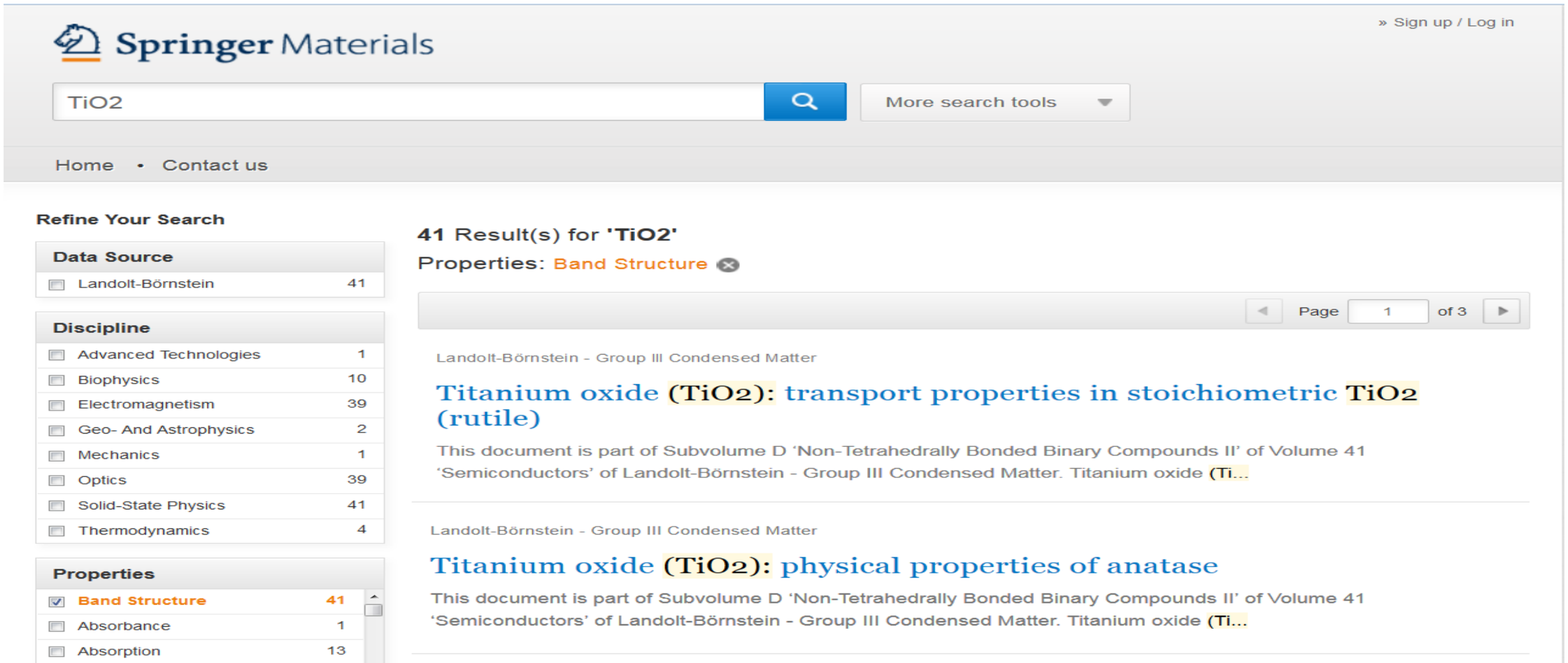

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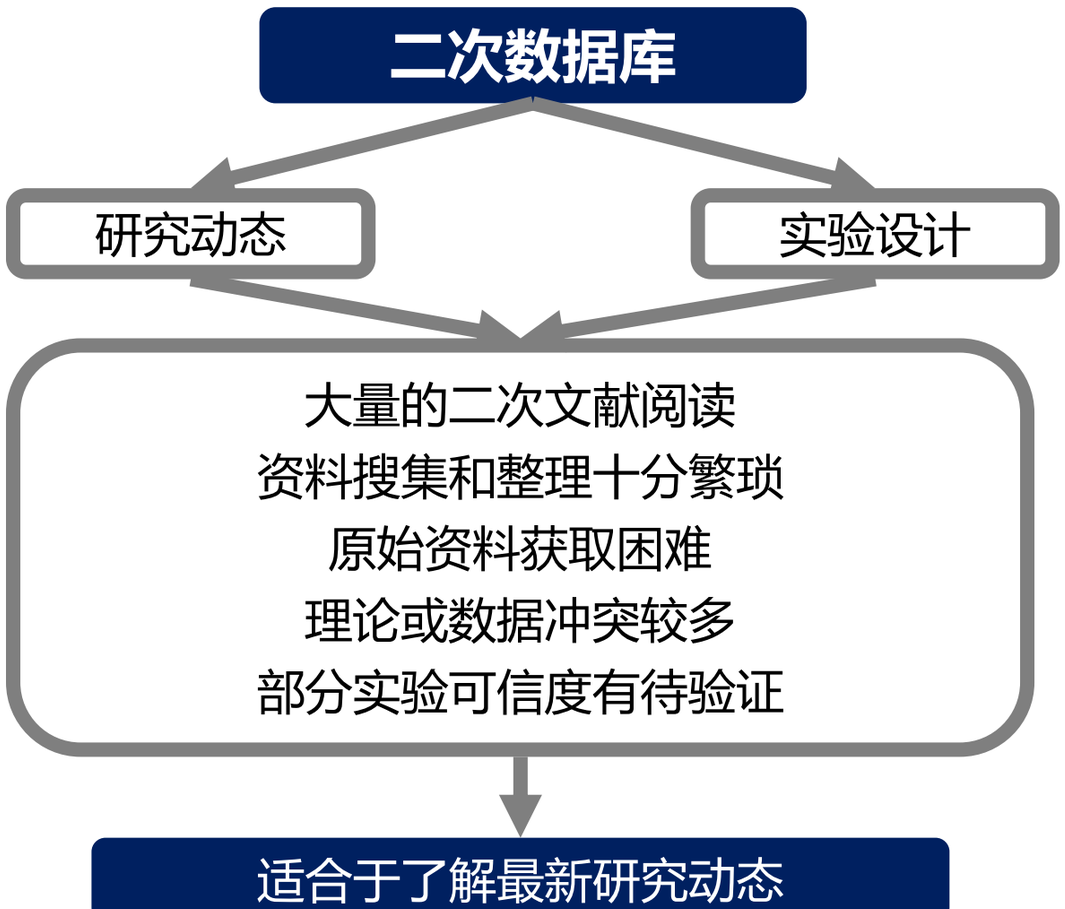

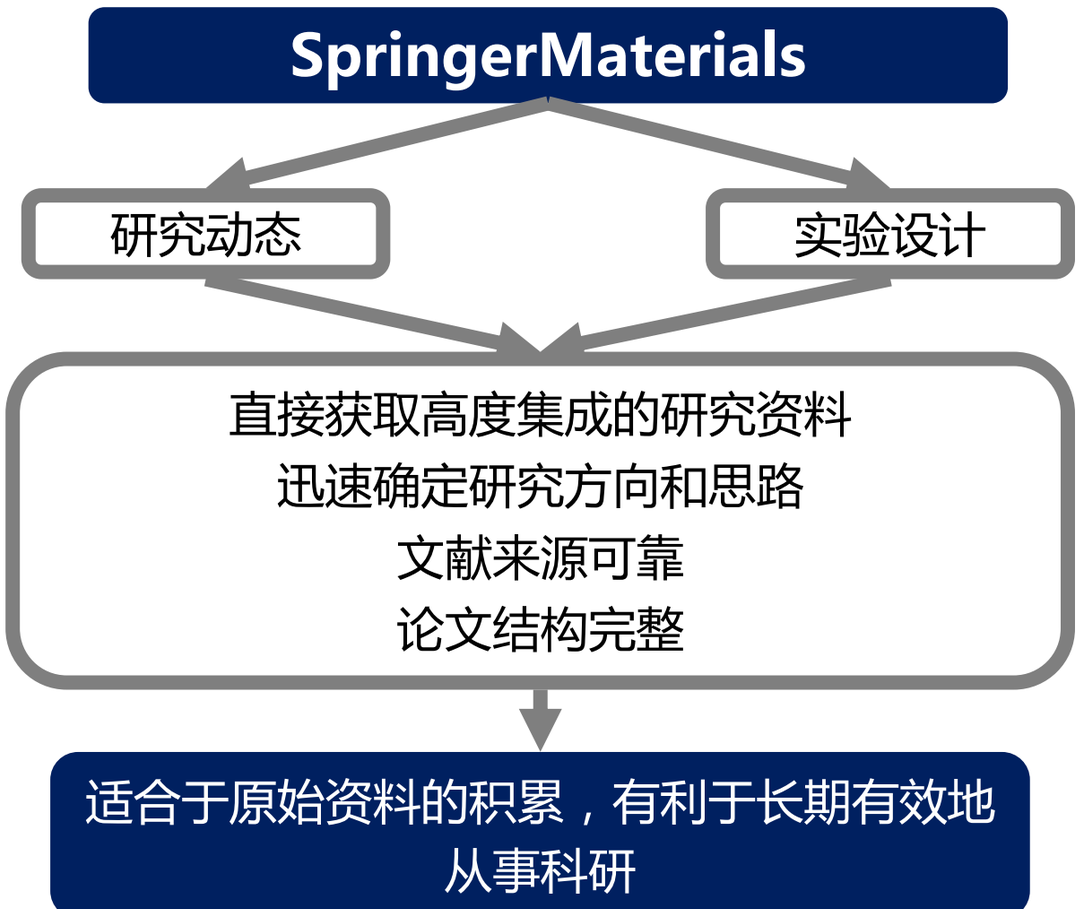

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- 可靠：所有数据均列明实验结果与其对应的测试方法，利于材料设计和实验检测分析
- 高效：各种辅助工具（精确坐标的相图、数据筛选的滑动条）提高信息获取效率

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