SLD Database

1.0 alpha

Query Database | Calculate SLD | Enter Material | Login | About

Field	search for value
Name	
Formula	
Description	
Submit	

SLD Database

1.0 alpha

Field	search for value
Name	
Formula	Fe
Description	
	Submit

Results of database query: Never Selected ORSO validated

	Id	Name	Description	Formula	Hr fomula	Density	Mu	Physical state	Tags	Ref website	Reference	Doi	Purity	Cas no	Crystal data	Temperature	Data origin	Comments
select	26	Iron		Fe		7.874	0.0	solid	[]	link	Python module periodictable, data source: ILL Neutron Data Booklet						text book	
select	103	Co20Fe60B20		B20Co20Fe60		5.629	1.68	solid	[]		Christy Kinane						unspecified	
select	178	FeO		FeO		5.745	0.0	solid	[]		Christy Kinane						unspecified	
select	211	FePt	(L10)	FePt		15.2	0.0	solid	[]		Christy Kinane						unspecified	
select	174	Fe2O3		Fe2O3		5.242	0.0	solid	[]		Christy Kinane						unspecified	
select	104	Co40Fe40B20		B20Co40Fe40		5.724	1.6	solid	[]		Christy Kinane						unspecified	
select	105	Co60Fe20B20		B20Co60Fe20		5.821	1.52	solid	[]		Christy Kinane						unspecified	
select	113	BiFe0.5Mn0.5O3		BiFe0.5Mn0.5O3		8.3	0.0	solid	[]		Christy Kinane						unspecified	
select	134	Co0.5Fe0.5Si		Co0.5Fe0.5Si		2.884	1.0	solid	[]		Christy Kinane						unspecified	
select	227	Abc	DEF	Fe2O3Pt	Bier	23.1	0.4	solid	['magnetic', 'metal alloy', 'inorganic']		123	abc	bad	1234	none	234.5	interferometry	This is a comment
select	106	Fe		Fe		7.874	2.2	solid	[]		Christy Kinane						unspecified	
select	144	FeF2		F2Fe		4.09	0.0	solid	[]		Christy Kinane						unspecified	
select	147	FeRh		FeRh		9.64685	0.0	solid	[]		Christy Kinane						unspecified	
select	158	Co28Fe28B14Ta30		B14Co28Fe28Ta30		7.04477	0.0	solid	[]		Christy Kinane						unspecified	
select	163	FeCo		CoFe		8.35562	2.0	solid	[]		Christy Kinane						unspecified	

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Field	search for value
Name	
Formula	
Description	
Submit	

Results of database query: Never Selected ORSO validated

	Id	Name	Description	Formula	Hr fomula	Density	Mu	Physical state	Tags	Ref website	Reference	Doi	Purity	Cas no	Crystal data	Temperature	Data origin	Comments	
select	26	Iron		Fe		7.874	0.0	solid	[]	link	Python module periodictable, data source: ILL Neutron Data Booklet						text book		validate
select	1	Hydrogen	T=-252.87	H		0.0708	0.0	liquid	[]	link	Python module periodictable, data source: ILL Neutron Data Booklet						text book		validate
select	103	Co20Fe60B20		B20Co20Fe60		5.629	1.68	solid	[]		Christy Kinane						unspecified		validate
select	178	FeO		FeO		5.745	0.0	solid	[]		Christy Kinane						unspecified		validate
select	211	FePt	(L10)	FePt		15.2	0.0	solid	[]		Christy Kinane						unspecified		validate
select	174	Fe2O3		Fe2O3		5.242	0.0	solid	[]		Christy Kinane						unspecified		validate
select	14	Silicon	T=25	Si		2.33	0.0	liquid	[]	link	Python module periodictable, data source: ILL Neutron Data Booklet						text book		validate
select	5	Boron		B		2.34	0.0	solid	[]	link	Python module periodictable, data source: ILL Neutron Data Booklet						text book		validate
select	212	IrO2		IrO2		11.66	0.0	solid	[]		Christy Kinane						unspecified		validate
											Python module periodictable								

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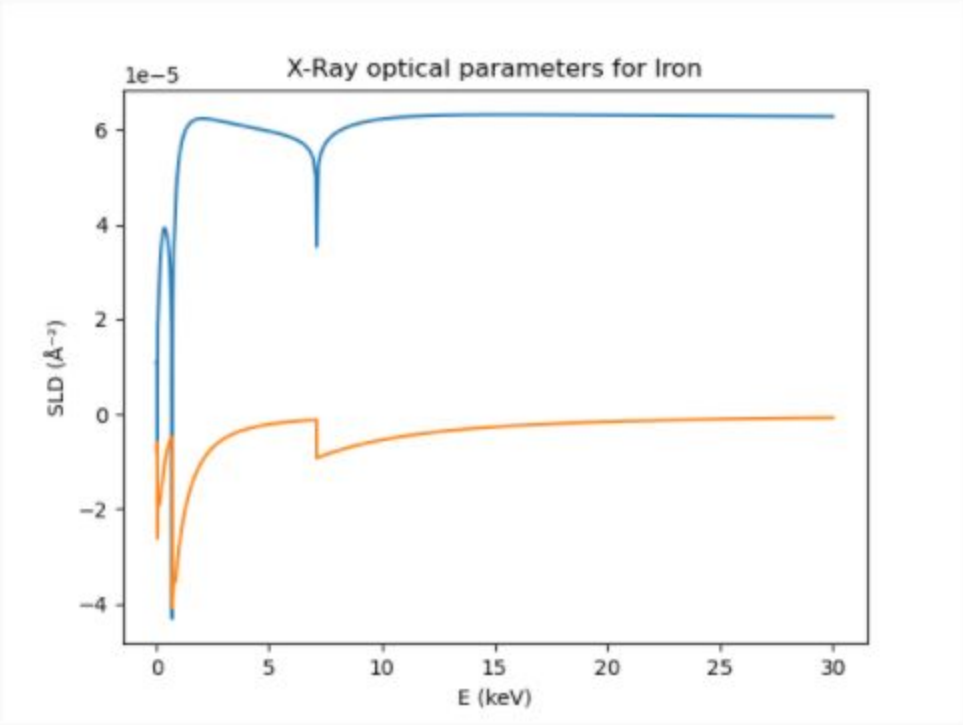
Field	value for calculation
Formula	Fe
Density (g/cm³)	7.873999999999997
Magnetisation (μB/FU)	0.0
Submit	

back to database query

Result of SLD calculation:

Compound	Iron	
Description		
Chemical Formula	Fe	
Density (g/cm³)	7.8740	
Neutron nuclear SLD (10^{-6} Å^{-2})	8.024054	-0.000604
Neutron magnetic SLD (10^{-6} Å^{-2})	0.000000	
Cu-Kα SLD (10^{-6} Å^{-2})	59.474664	-7.678323
Mo-Kα SLD (10^{-6} Å^{-2})	63.068248	-2.023148
Custom Energy (eV)	SLD (10^{-6} Å^{-2})	
8040		



SLD Database

1.0 alpha

name	
description	
formula	exmpl: Fe2O3 / H[2]2O
HR_fomula	
density	0.0<value<None
FU_volume	0.0<value<None
SLD_n	complex: (real)+(imag)j
SLD_x	complex: (real)+(imag)j
E_x	
mu	
physical_state	solid
tags	magnetic polymer biology membrane
ref_website	exmpl: http://www.google.cor
reference	
doi	
purity	
CAS_No	
crystal_data	
temperature	0.0<value<None
data_origin	unspecified
comments	
Submit	

SLD Database

1.0 alpha

This is a database for materials for scattering length density (SLD) calculations for neutron and x-ray reflectometry and small angle scattering. It is provided by the Open Reflectometry Standards Organization (ORDO):
ORSO Website

In addition to this website manual search we provide a simple API for that can be called by other software and provides data as JSON text.

Usage:

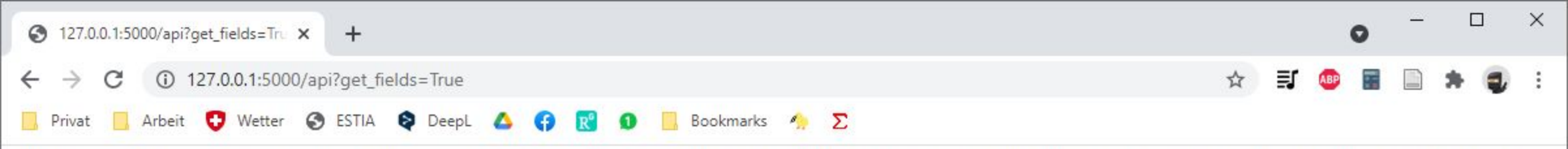
Manual calculation of SLD form formula and density values:
https://{this website}/api?formula={}&density={}&sldcalc=true

Retrieve a list of fields that can be used for database queries.
https://{this website}/api?get_fields=True

Search database for material using arbitrary fields.
https://{this website}/api?field1={}&field2={}

Calculation of SLD form database material.
https://{this website}/api?ID={}:

Download Python API



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127.0.0.1:5000/api?ID=174

Privat Arbeit Wetter ESTIA DeepL Bookmarks

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In [1]:
```
%pylab inline
from slddb import api
```

```
Populating the interactive namespace from numpy and matplotlib
```

In [2]:
```
results=api.search(formula='Si')
print(", ".join(results[0].keys())+"\n")
for ri in results:
    print(ri['ID'], ri['name'], ri['formula'], ri['description'], ri['validated'], ri['validated_by'])
```

```
ID, created, updated, validated, validated_by, accessed, selected, name, description, formula, HR_fomula, density, FU_volume, S
LD_n, SLD_x, E_x, mu, physical_state, tags, ref_website, reference, doi, purity, CAS_No, crystal_data, temperature, data_origi
n, comments

14 Silicon Si T=25 2021-04-12 20:16:55 Artur Glavic <artur.glavic@psi.ch>
93 Si Si None None None
118 SiO2 O2Si fused SiO2 (Quartz) None None
220 InAs AsIn None 2021-05-21 10:45:23 Artur Glavic <artur.glavic@psi.ch>
134 Co0.5Fe0.5Si Co0.5Fe0.5Si None None None
98 SiO2 O2Si Native Oxyde None None
```

In [3]:
```
material=api.material(ID=14)
material
```

Out[3]:
```
Material([('Si', 1.0)], fu_volume=20.015910254527896)
```

In [4]:
```
material.rho_n
```

Out[4]:
```
(2.0737053410104337e-06-2.3757518571628716e-11j)
```

In [5]:
```
material.fu_dens
```

Out[5]:
```
0.04996025598055353
```

In [6]:
```
material.dens
```

Out[6]:
```
2.33
```

In [7]:
```
material.delta_of_E(8.047823)
```

Out[7]:
```
(2.007024433211989e-05-4.574332903661553e-07j)
```