MPOD: a Matrial Property Open Database related to Structural information

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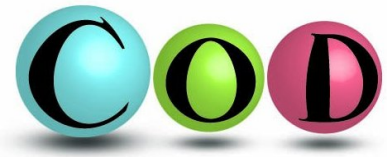


- Introduction

Data are arriving in ever increasing rates. Thus, automated software tools are needed to cope with the growing amount of data, to provide consistent, uniform and accurate information: **> 155000** cif files

The following goals are set by COD team:

- build automated structure deposition tools;
- build a collaboration platform for structure validation and curation;
- ensure data quality – uniformity, integrity, and trustworthiness;
- make scientific data freely accessible to anyone.

Deposit your data to COD for publication!

http://www.crystallography.net/

Crystallography Open Database
Validation and Deposition Interface

Select CIF file for check:
/home/saulius/ALL.CIF Browse...
Validate

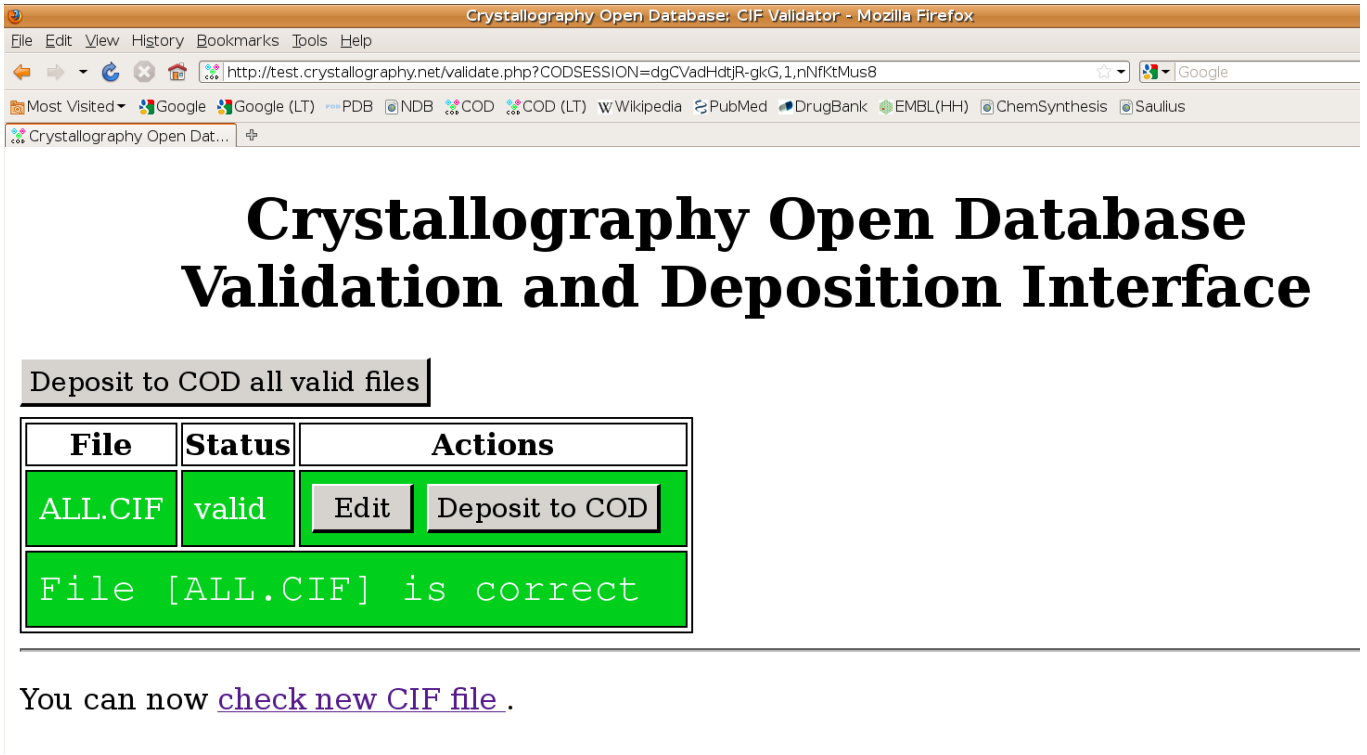
About this Validation Interface

This interface allows you to upload, validate and edit CIF files before submitting them for deposition.

Steps

The process of files deposition, after you have uploaded your data is prettty simple.
First step, after files have been uploaded, is validation. Our scripts performs some validation. Results are displayed to you next to your files.

COD - Automatic data deposition



Expanding the PCOD

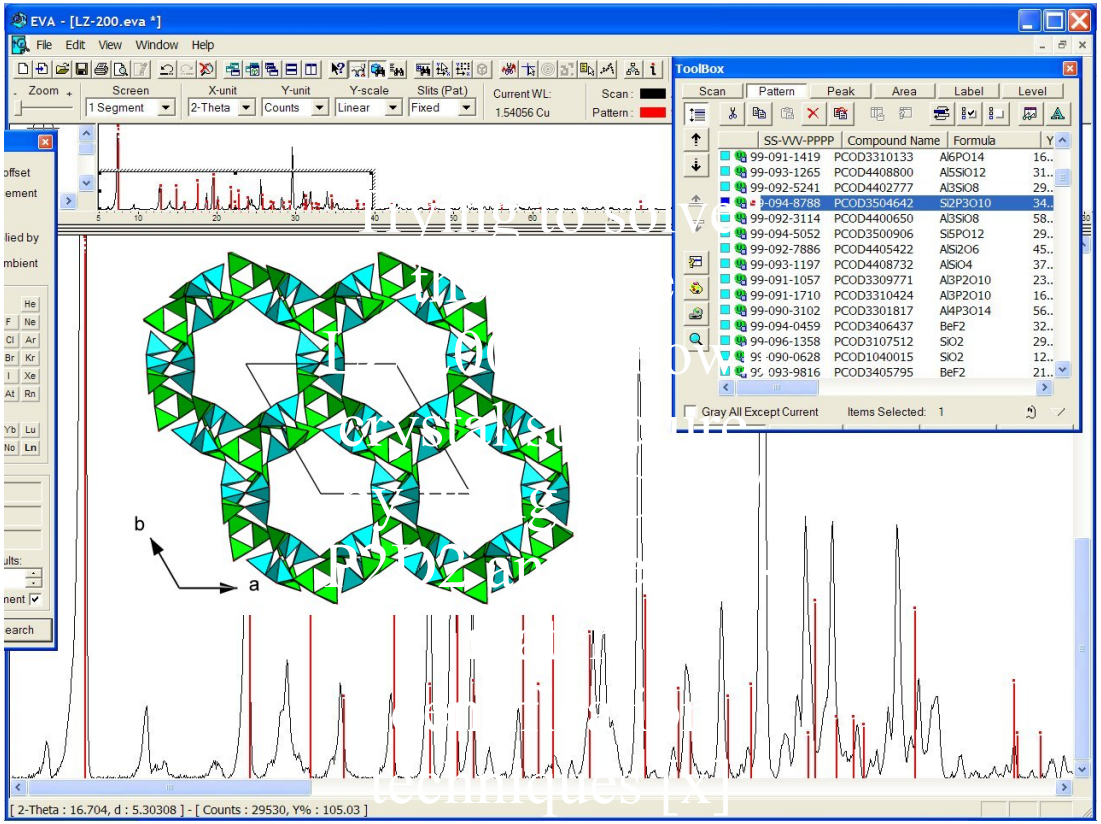
2011 state: 898.707 SiO_2 entries were added from *ZEFSAII* zeolite predictions and the contributions from *GRINSP* increased to 163.520 (silicates, phosphates, sulfates of Al, Ti, V, Ga, Nb, Zr, or zeolites, fluorides, etc). The PCOD is the first database to attain and offer **more than one million of CIF entries**.

Software : a new *GRINSP* version is now available [3] for parallel computing (for instance using fully the 8 processors of an INTEL core i7).

Other data from other prediction computer programs (*CASTEP*, *CERIUS2*, *CRYSTAL*, *G42*, *GULP*, *USPEX*…) are expected, just send them, please.

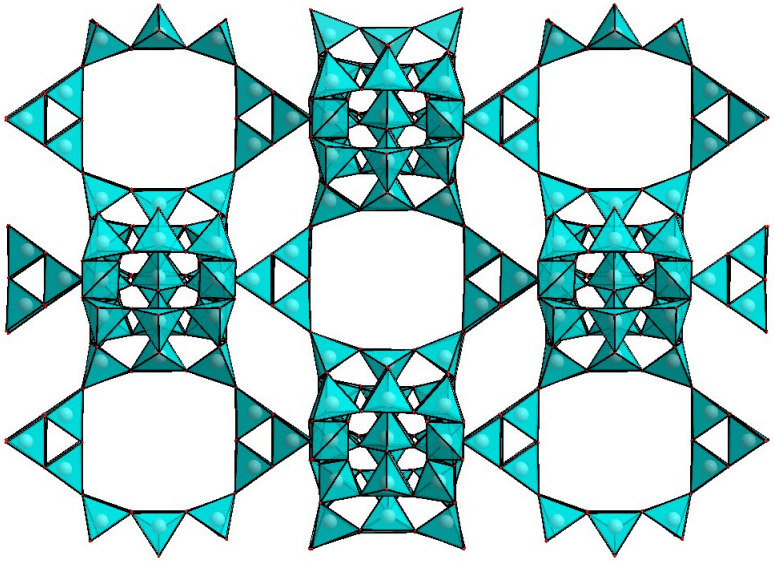
PCOD Powder P2D2

All powder patterns (> 1 million) were calculated and gathered in the P2D2 (Predicted Powder Diffraction Database [4]), they can be used for search-match purposes with *EVA* (Bruker), *Highscore* (Panalytical) and more soon.

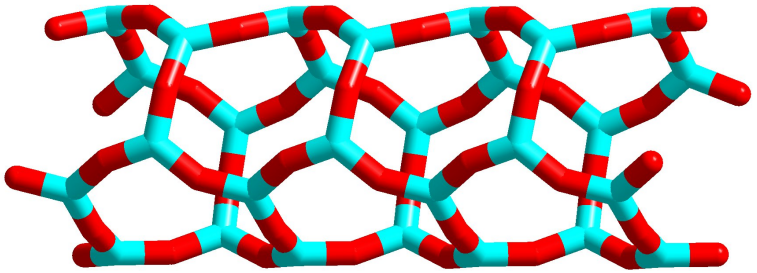


VIRTUAL MODELS in PCOD

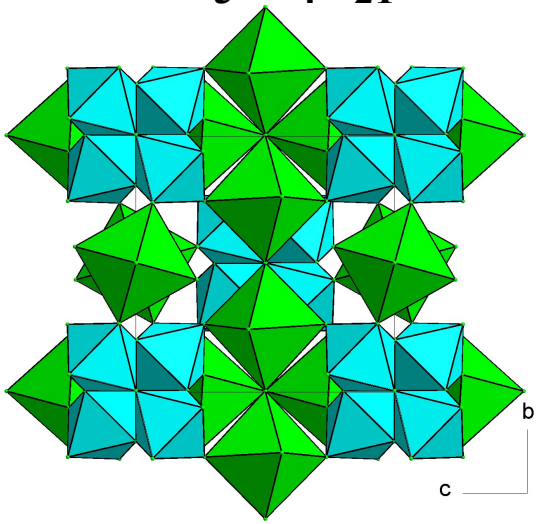
Zeolites



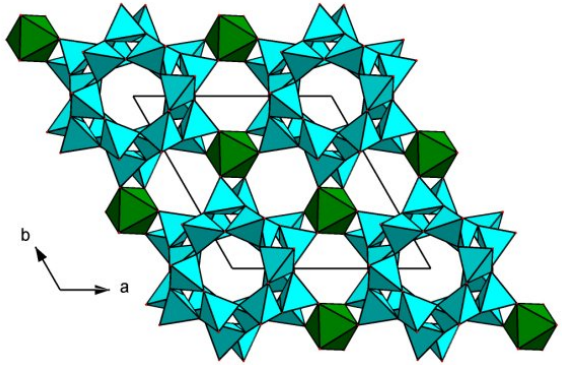
B_2O_3 nanotubes



$[Ca_3Al_4F_{21}]^{3-}$



Titanosilicates



MPOD
Material Property Open Database
www.materialproperties.org

- Inspired by COD, MPOD
- Collect and make open mode published material properties data
- Keeping connection to the structural information
- New cif-compliant .MPOD files
- Search tool
- Online view of tensors
- Publication references

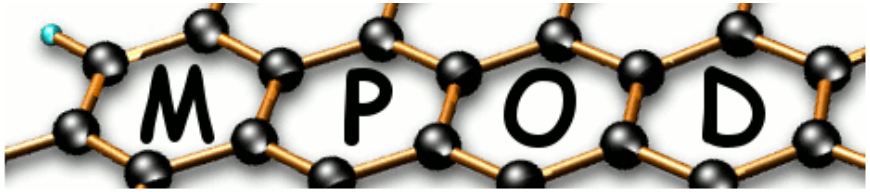
Coded Properties

- elastic stiffness and compliance
- internal friction
- resistivity
- dielectric permittivity and stiffness
- heat capacity
- thermal conductivity, diffusivity and expansion
- piezoelectricity, electrostriction, electromechanical coupling
- piezooptic, photoelastic
- superconducting critical fields, penetration and coherence lengths

Original published paper serves as reference
Experimental information is given
One mpod file for one publication and one phase.

Coding

- Uses a Starfile syntax: developed for the Crystallographic Information Files (CIF)
- Structural information in the CORE CIF dictionary
- New dictionary for properties in Dictionary Definition Language DDL1
- Some tricks were adopted to adapt vs Starfile syntax
- Units are univocally define in the dictionary itself
- Experimental conditions (temperature, pressure, …) are inserted
- All non-zero components explicitly written
- Diagonally symmetric components not repeated



Material Properties Open Database

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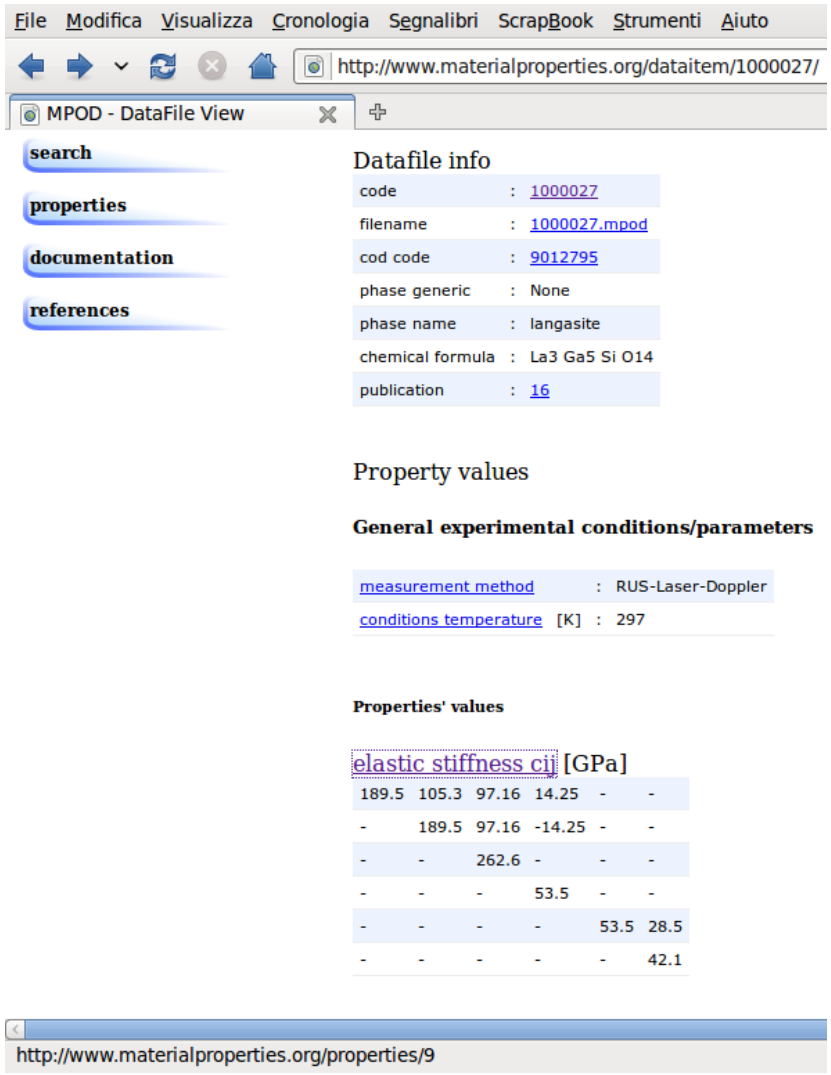
Input search parameters

Phase Name: aluminum
Formula contains:
COD code:
Publication author: Submit

Search results:

Found datafiles

code	filename	cod code	phase generic	phase name	chemical formula	publication
1000002	1000002.mpod	9008460	None	aluminum	Al	2
1000003	1000003.mpod	9008460	None	aluminum	Al	3
1000093	1000093.mpod	9008460	None	Aluminum	Al N	53
1000094	1000094.mpod	9008860	None	Aluminum nitride	Al N	54



Datafile info

code	:	1000069
filename	:	1000069.mpod
cod code	:	1010458
phase generic	:	KDP
phase name	:	Mn-doped potassium dihydrogen phosphate
chemical formula	:	
publication	:	37

Property values

Other experimental conditions/parameters

measurement method [n.a.] : XRD

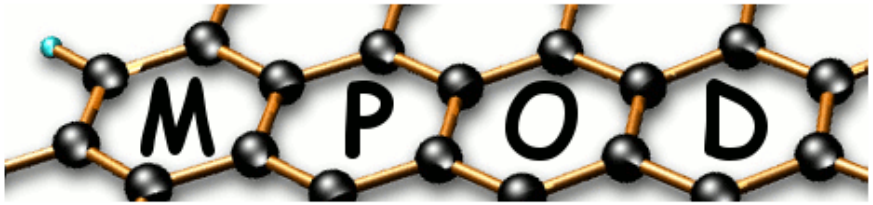
Properties' values

piezoelectric dij [m.V^-1]

-	-	-	2.3(1)	-	-
-	-	-	-	2.3(1)	-
-	-	-	-	-	47(2)

```
data_1000280
_cod_database_code              2101499
_structure_refined 'no'
_phase_name 'diamond'
_chemical_formula 'C'
_chemical_formula_sum 'C'
_symmetry_point_group_name_H-M 'm -3 m'
_cell_length_a  3.56658
_cell_length_b  3.56658
_cell_length_c  3.56658
_cell_angle_alpha  90
_cell_angle_beta   90
_cell_angle_gamma  90
loop_
_publ_author_name
'Ramachandran, G.N.'
_publ_section_title
;
 Photoelastic constants of diamond
;
_journal_name_full              'Proceedings of the Indian Academy of Sciences A'
```

```
_journal_volume                  25
_journal_issue                   ?
_journal_page_first              208
_journal_page_last               219
_journal_year                    1947
_phase_density ?
_prop_measurement_method 'Birefringence'
_prop_conditions_wavelength 0.5893
_prop_photoelastic_pij 'pij'
_prop_piezooptic_piij 'piij'
loop_
_prop_data_label
_prop_data_tensorial_index
_prop_data_value
pij 11 0.12(5)
pij 12 -0.32(5)
pij 13 -0.32(5)
pij 21 -0.32(5)
pij 22 0.12(5)
pij 23 -0.32(5)
pij 31 -0.32(5)
pij 32 -0.32(5)
pij 33 0.12(5)
```



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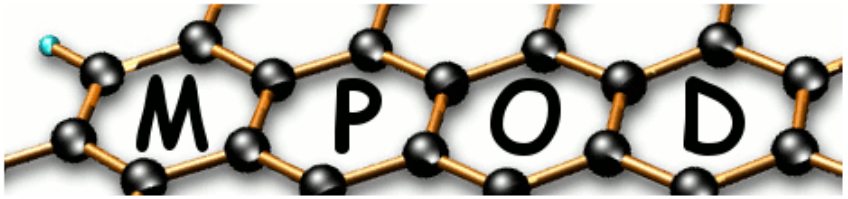
Publication details

title	Anisotropy of the superconducting state parameters and intrinsic pinning in low-level Pr-doped YBa2Cu3O7-d single crystals
authors	Kortyka, A.; Puzniak, R.; Wisniewski, A.; Zehetmayer, M.; Weber, H.W.; Cai, Y.Q.; Yao, X.
journal	Superconductor Science and Technology
year	2010
volume	23
issue	10
first page	None
last page	None
reference	065001
pages number	7

Associated datafiles

code	filename	cod code	phase generic	phase name	chemical formula	publication
1000107	1000107.mpod	None	None	YBCO	Y Ba2 Cu3 O6.915	65



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Property details

tag	_prop_superconducting_critical_field2_Hc2i
name	prop superconducting critical field2 Hc2i
description	_superconducting_critical_field2_Hc2i
tensor dimensions	3
units	T
units detail	tesla

Associated datafiles

code	filename	cod code	phase generic	phase name	chemical formula	publication
1000097	1000097.mpod	9088326	None	LiFeAs	Li Fe As	56
1000102	1000102.mpod	None	?	iron arsenide	Ba Fe2 As1.3 P0.7	60
1000107	1000107.mpod	None	None	YBCO	Y Ba2 Cu3 O6.915	65
1000108	1000108.mpod	None	None	YBCO	Y Ba2 Cu3 O6.973	65
1000109	1000109.mpod	None	None	Pr-YBCO	Y0.992 Pr0.008 Ba2 Cu3 O6.934	65

Acknowledgments

- Vilnius COD development group: Research Council of Lithuania, contract No. MIP-124/2010
- all CIF donators, listed on our Web page, numerous anonymous volunteers who help to collect data and keep COD running
- Commercial supporters for donation (hardware and financial support)
- Xmat project (“Combination of X-Ray diffraction and X-Ray Fluorescence techniques in material science”), supported by the Provincia Autonoma di Trento and the European Union in the framework of the Marie Curie COFUND program - Call for proposals 4 - researcher 2009 – Outgoing.