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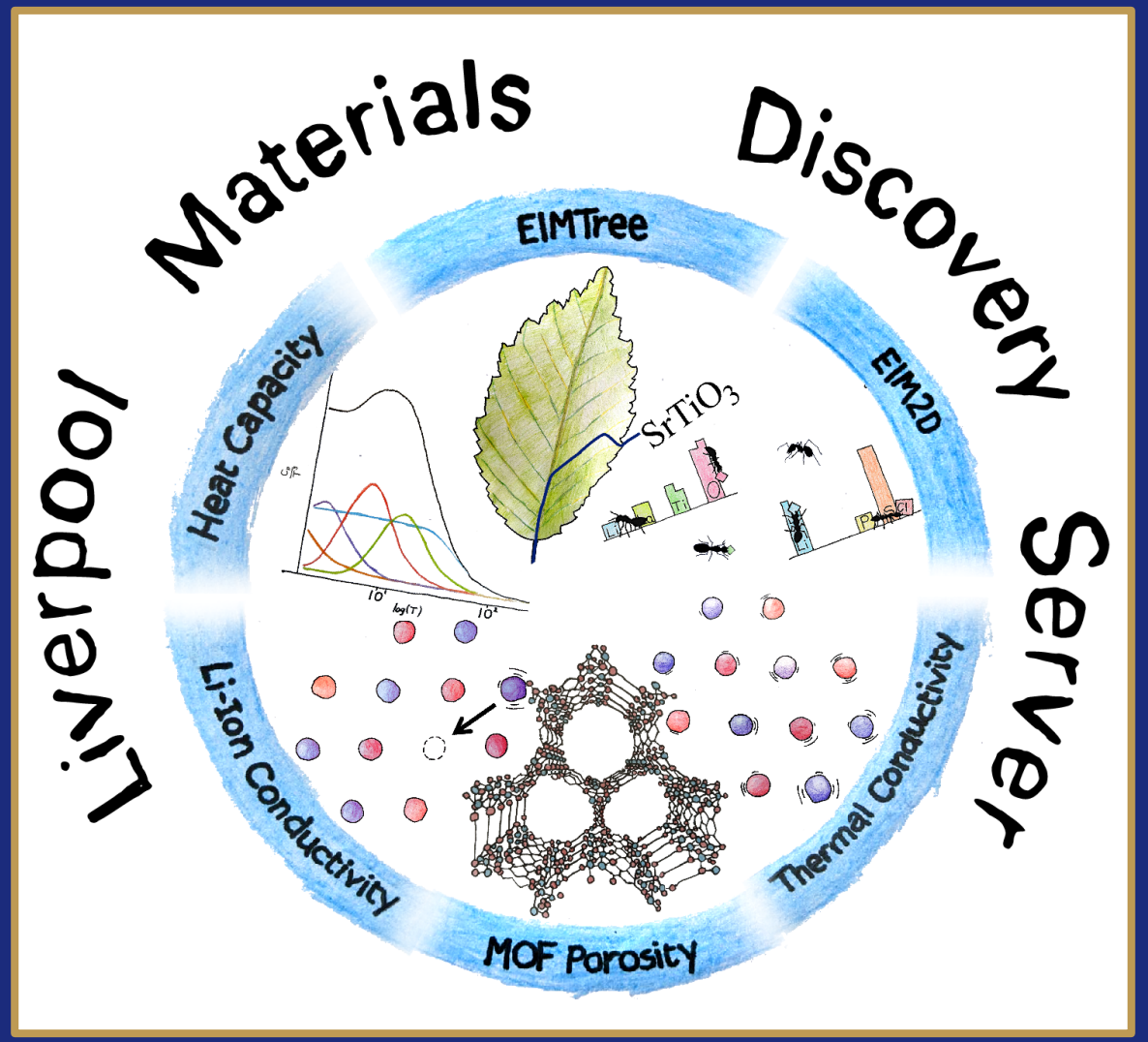
The Liverpool Materials Discovery Server: Background and Application

Matthew S Dyer
Department of Chemistry
University of Liverpool

Le Studium, Orléans, 5/10/2023

https://lmds.liverpool.ac.uk

Sam Durdy



Cameron Hargreaves

S Durdy, C J Hargreaves, *et al*., *Digital Discovery* (2023) *Accepted*

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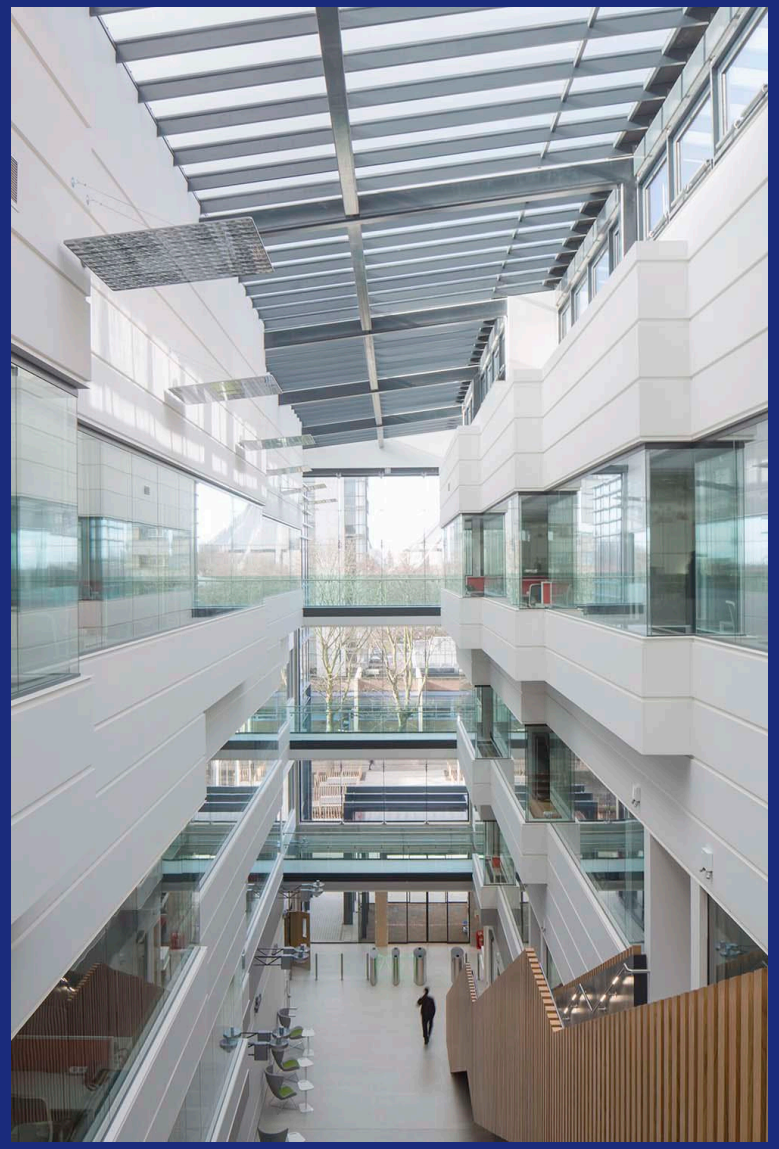
The Research Environment



- The Materials Innovation Factory (MIF) enables chemists, physicists, mathematicians and computer scientists to work together on a single site.
- The Leverhulme Research Centre for Functional Materials Design funds researchers and PhD students to work in this interdisciplinary space.
- Resulting in new approaches to aid discovery of novel materials.

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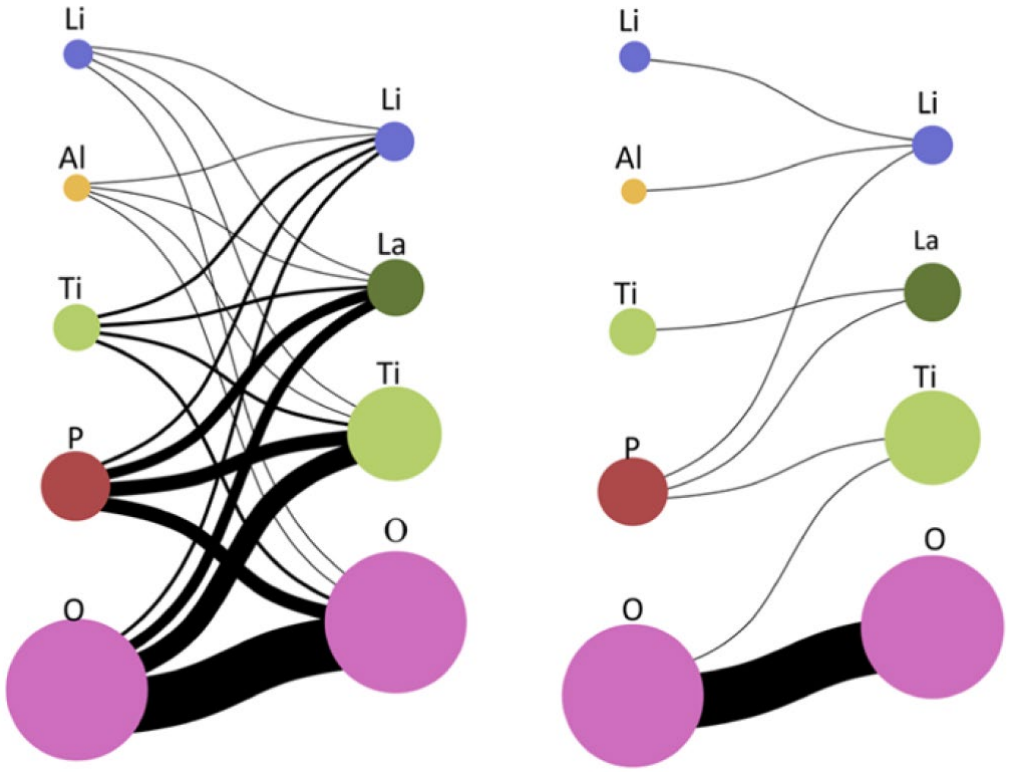
The Element Movers Distance

$Li_{0.7}Al_{1.3}Ti_{0.7}(PO_4)_3$ $La_{0.57}Li_{0.29}TiO_3$



All solutions

Optimal solution

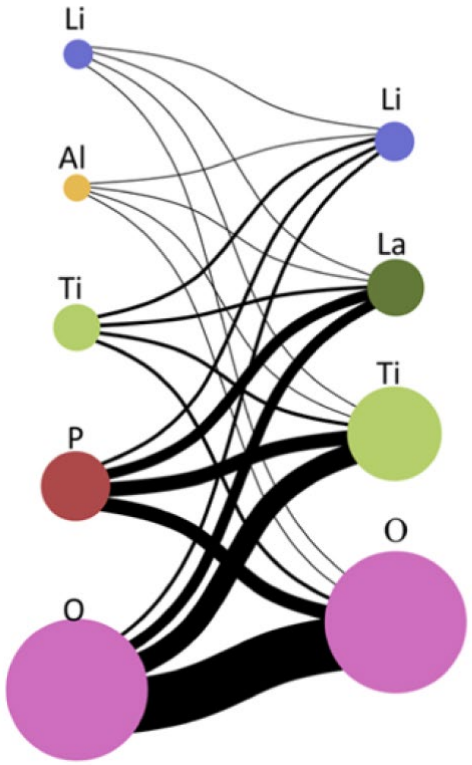
ElMD = 12.7

- We needed a quantitative measure of chemical similarity between two compositions
- We use the Earth Movers Distance
- Elements are labelled with their Pettifor number
- We seek the transfer elements from one to the other with the lowest total work done – the EIMD

C J Hargreaves, et al., *Chem. Mater.* 32 (2020) 10610

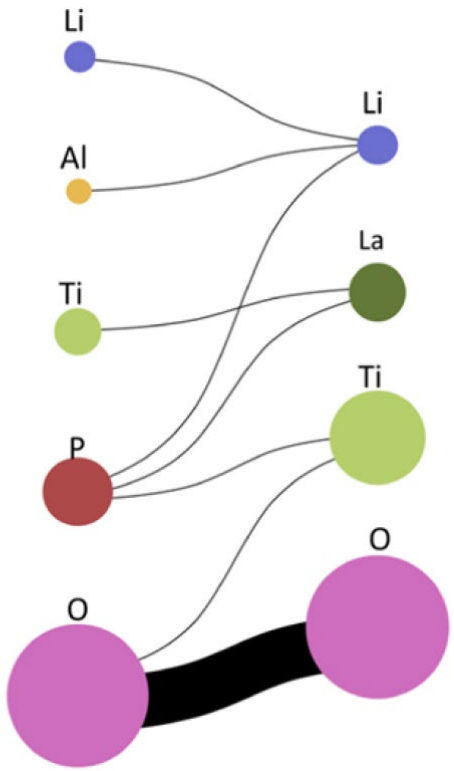
The Element Mover's Distance

$Li_{0.7}Al_{1.3}Ti_{0.7}(PO_4)_3$



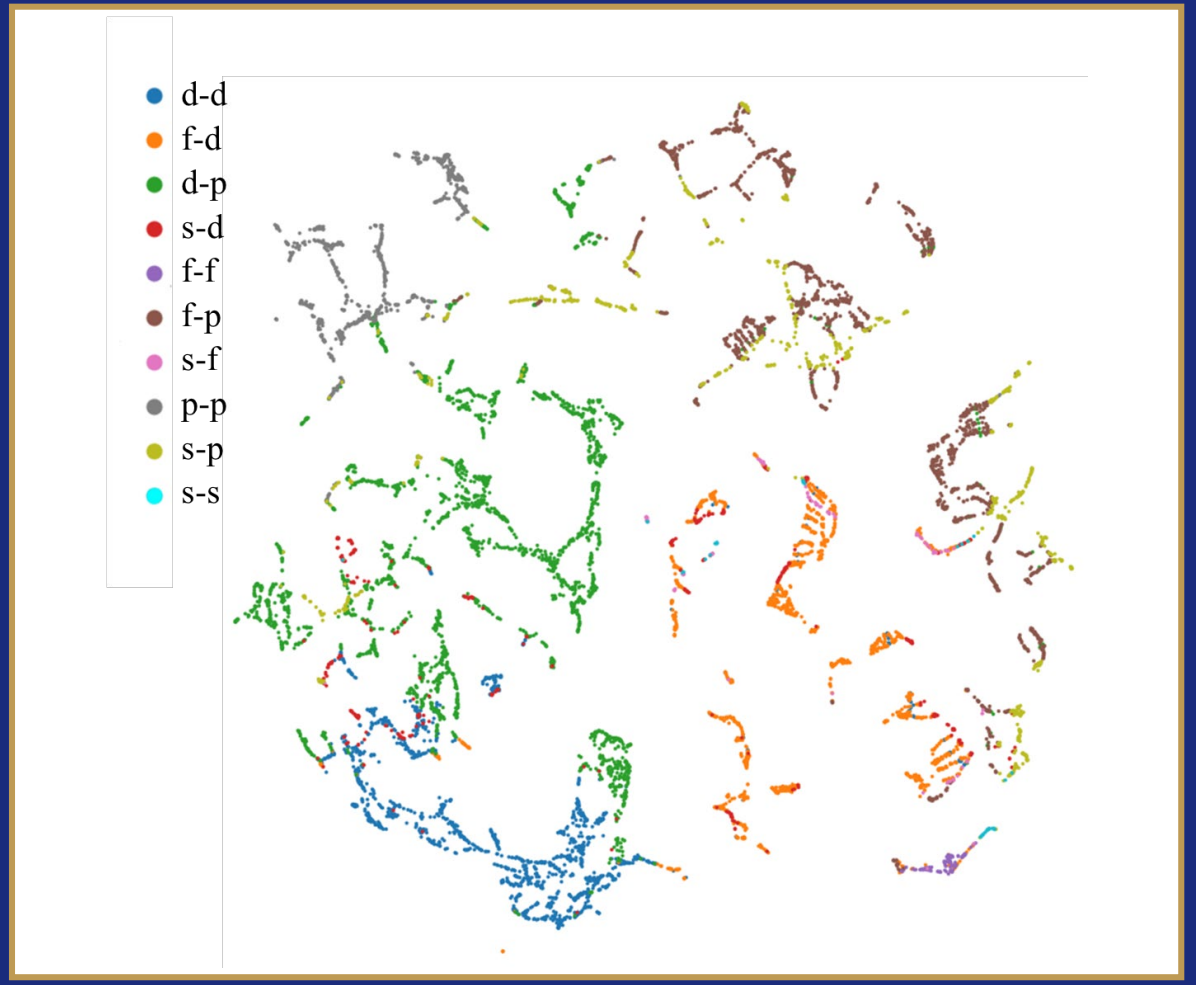
All solutions

$La_{0.57}Li_{0.29}TiO_3$

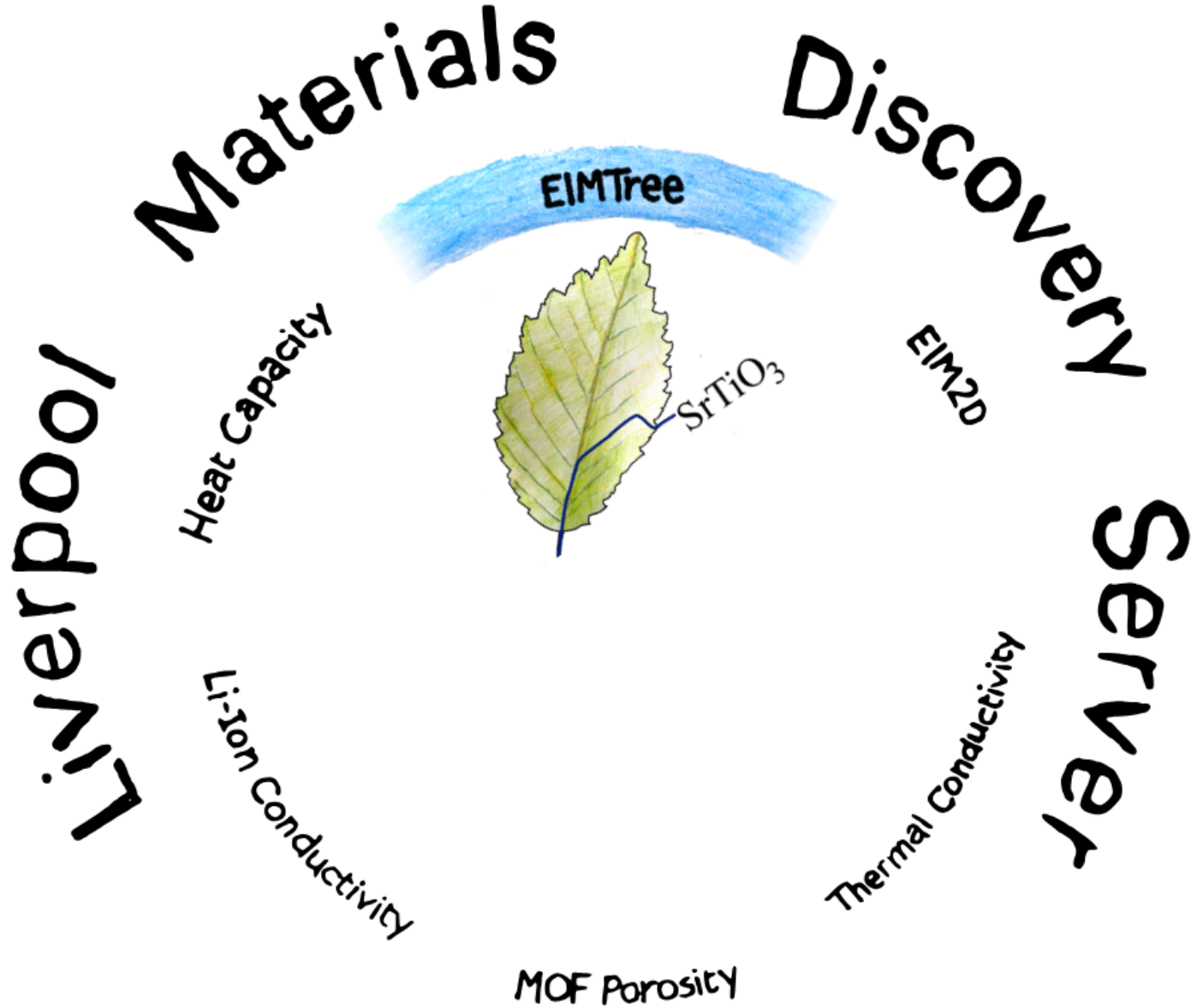


Optimal solution

ElMD = 12.7



C J Hargreaves, et al., *Chem. Mater.* 32 (2020) 10610



Search the largest repositories of reported materials for compounds of interest using the chemical composition

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Liverpool Materials Discovery Server LMDS

ElMTree

Enter a chemical composition to see the 100 most similar ElMTree indexed compositions, the databases these are reported in with their associated IDs, and the ElMD distance to the query. This application was reported in The Liverpool Materials Discovery Server: A suite of tools for the collaborative discovery of materials, and implements the process described in The Earth Movers Distance as a Metric for the space of Inorganic Compositions. Please consider citing these papers if you use this in your work.

If you would like to access this tool using an API please click here for more information

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Liverpool Materials Discovery Server LMDS

ElMTree

MgSiO3

Enter a chemical composition to see the 100 most similar ElMTree indexed compositions, the databases these are reported in with their associated IDs, and the ElMD distance to the query. This application was reported in The Liverpool Materials Discovery Server: A suite of tools for the collaborative discovery of materials, and implements the process described in The Earth Movers Distance as a Metric for the space of Inorganic Compositions. Please consider citing these papers if you use this in your work.

If you would like to access this tool using an API please click here for more information

ElMTree

MgSiO3

Searched 1,367,526 unique compositions across 5,410,119 records for $Mg_{0.2}$ $Si_{0.2}$ $O_{0.6}$ in 0.044s

Refine Search

Composition	Database: Matched IDs	Distance
$Mg_{0.2}$ $Si_{0.2}$ $O_{0.6}$ 	MC 3D: 355659, 286755, 197969, 288960, 286091, 121980, 92458, 443473, 287831, 67294, 299292, 356152,... ICSD: 290217, 68370, 290220, 34074, 31288, 37313, 171911, 30808, 31176, 137833, 80669, 64629, 290216,... Pearsons: 1247033, 1247034, 1247031, 1247036, 1247035, 1247032, 1213086, 1221853, 1247037, 1720923,... MPDS Structural Database: S1247033, S1247034, S1247031, S1247036, S1247035, S1247032, S1213086, S1221853, S1247037,... MPDS Property Database: P11803448, P11324227, P20004039, P1001007, P1800098, P1800348, P11324223,... Matbench Experimental Formation Enthalpy Kingsbury: 439 Brgoch Superhard Dataset: 2107 AFLOW: 0f52c618e87867cc, 1d7e4e940b42e292, 2ba30825febc0878, 8f13cdb0337ad6f5, 82d6b67054d0c51d,... Alexandria: agm003248137, agm002561439, agm003274640, agm003272733, agm003227041, agm003248089 The Materials Project: mp-1180468, mp-657338, mp-644879, mp-1020125, mp-1182302, mp-603930, mp-554137, mp-... OMDB: 39549, 35 2DMatpedia: 2dm-4459 ICSD Theoretical: 5225, 159559, 159563, 159564, 680702, 5218, 163892, 5300, 674100, 163891, 151950, 159514,... Wolverton Oxides: 2251, 3626 Jarvis ML: 11184, 11712, 12277, 12487, 15884, 20208, 24066, 24263 Castelli Perovskites Dataset: 9276, 15213 Matbench log gvrh v0.1: 7445, 8275, 8301, 8372, 10754 Jarvis 3D: 11312, 11882, 12448, 12657, 16170, 20662, 24636, 24834 Matbench log kvrh v0.1: 7445, 8275, 8301, 8372, 10754 Matbench log gvrh v0.1: 9276, 15213 Matbench Dielectric: 3427	0.0
$Mg_{0.196}$ $Zn_{0.004}$ $Si_{0.2}$ $O_{0.6}$	MPDS Structural Database: S1047271, S1047268 Pearsons: 1047271, 1047268	0.004

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Liverpool Materials Discovery Server LMDS

ElMTree

Li7SiO5Cl

Enter a chemical composition to see the 100 most similar ElMTree indexed compositions, the databases these are reported in with their associated IDs, and the ElMD distance to the query. This application was reported in The Liverpool Materials Discovery Server: A suite of tools for the collaborative discovery of materials, and implements the process described in The Earth Movers Distance as a Metric for the space of Inorganic Compositions. Please consider citing these papers if you use this in your work.

If you would like to access this tool using an API please click here for more information

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Liverpool Materials Discovery Server LMDS

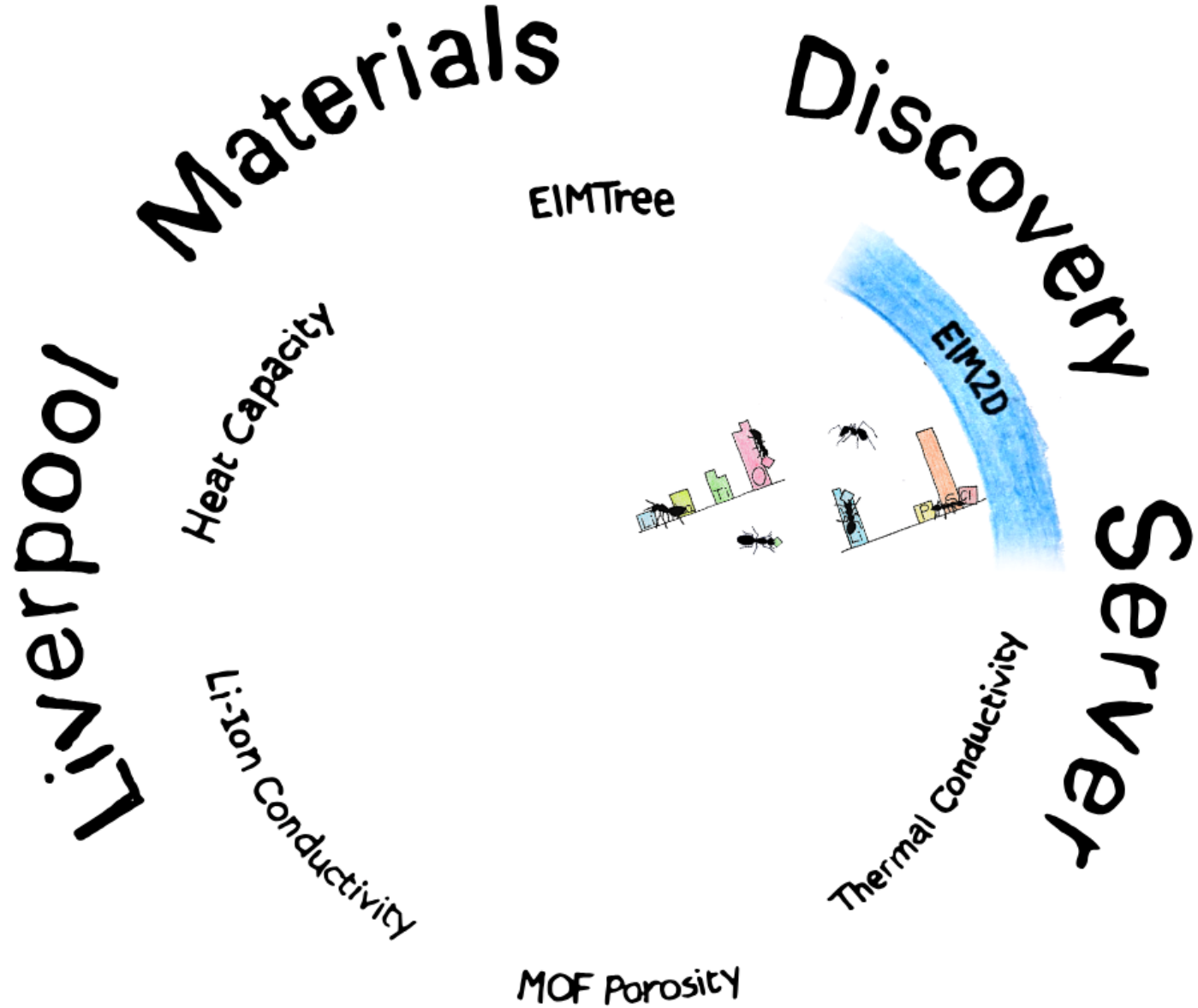
ElMTree

Li7SiO5Cl

Searched 1,367,526 unique compositions across 5,410,119 records for $Li_{0.5}$ $Si_{0.071}$ $O_{0.357}$ $Cl_{0.071}$ in 0.067s

Refine Search

Composition	Database: Matched IDs	Distance
$Li_{0.5}$ $Sn_{0.083}$ $O_{0.417}$ 	MPDS Structural Database: S1834891	0.595
$Li_{0.5}$ $B_{0.1}$ $O_{0.4}$ 	Alexandria: agm003225142, agm003281557 The Materials Project: mp-768960, mp-768966, mp-768967, mp-755346 Jarvis ML: 21977 Jarvis 3D: 22482	0.671
$Li_{0.5}$ $Bi_{0.071}$ $O_{0.429}$ 	MC 3D: 426306 ICSD: 155950 Pearsons: 1818766, 1121989 MPDS Structural Database: S1818766, S1121989 MPDS Property Database: P1128474, P20057326, P1128479, P20103788 Alexandria: agm003215469, agm003215470 The Materials Project: mp-38487, mp-754060 Jarvis ML: 3407 Jarvis 3D: 3453	0.786
$Li_{0.496}$ $Ge_{0.065}$ $P_{0.007}$ $S_{0.36}$ $I_{0.072}$	MPDS Structural Database: S1046127 Pearsons: 1046127	0.883



Enter a single composition to see it within the context of reported compositions or generate ElM2D plots and distance matrices from lists of comma separated compositions

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Liverpool Materials Discovery Server LMDS

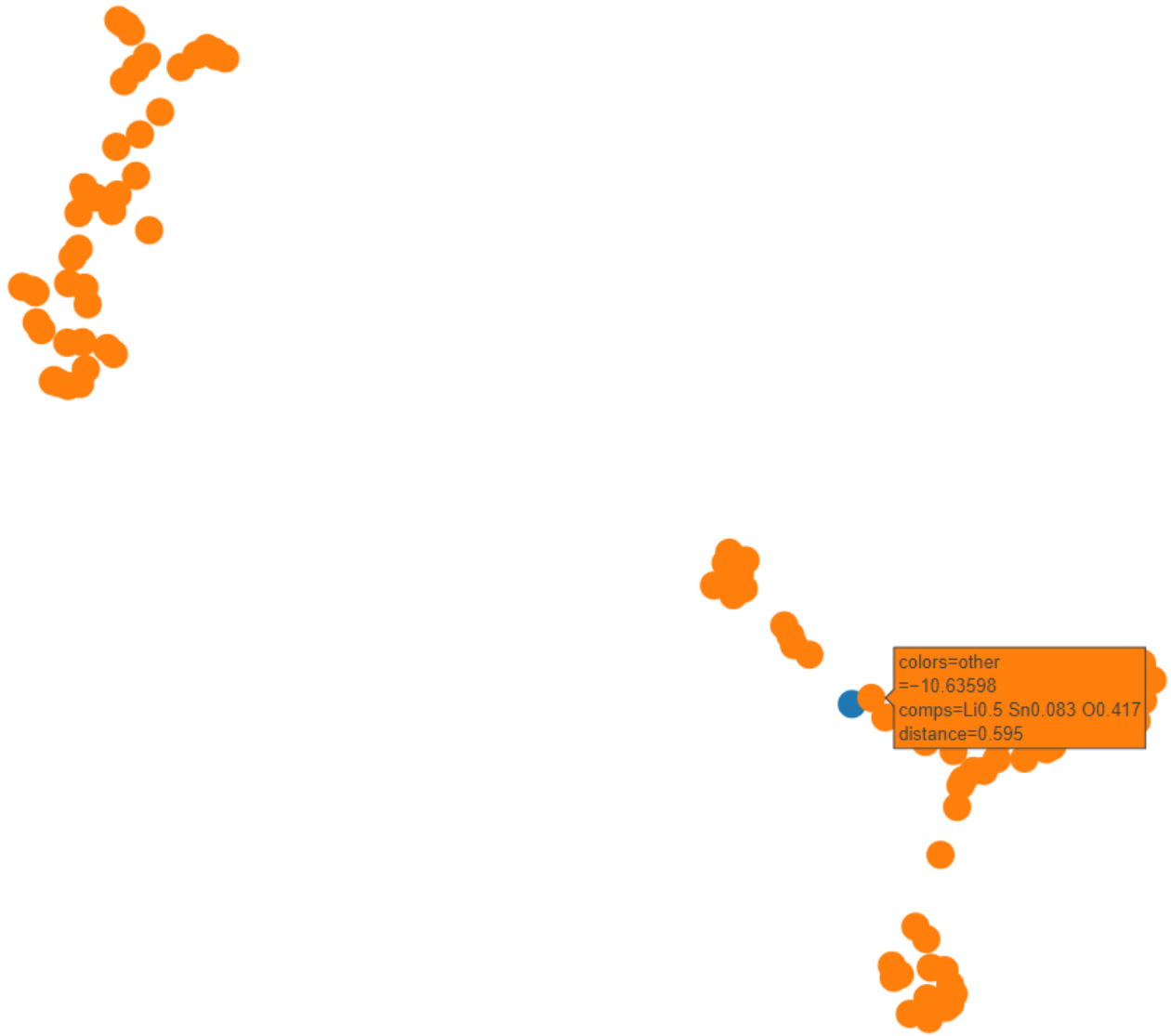
ElM2D

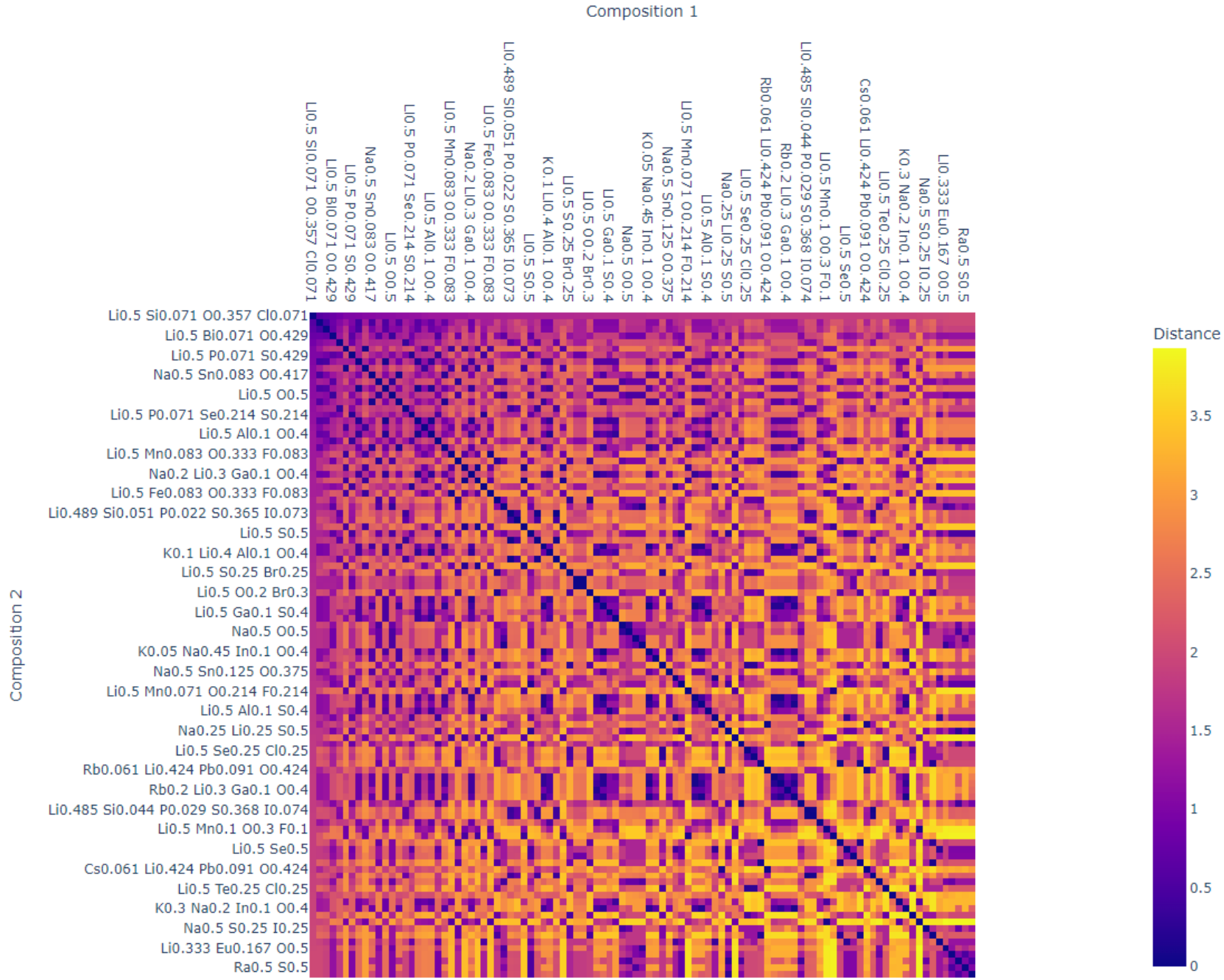
Li7SiO5Cl

Enter a composition to see the 100 most similar ElMTree indexed compositions, embedded to two dimensions via UMAP. Enter up to 100 compositions, separated via commas, to plot their chemical similarity. Tap the distance matrix to view specific distances. This application was reported in The Liverpool Materials Discovery Server: A suite of tools for the collaborative discovery of materials, and implements the process described in The Earth Movers Distance as a Metric for the space of Inorganic Compositions. Please consider citing these papers if you use this in your work.

EIM2D

Li7SiO5Cl




Composition 1
Composition 2
Distance
Li0.5 Si0.071 O0.357 Cl0.071
Li0.5 Bi0.071 O0.429
Li0.5 P0.071 S0.429
Na0.5 Sn0.083 O0.417
Li0.5 O0.5
Li0.5 P0.071 Se0.214 S0.214
Li0.5 Al0.1 O0.4
Li0.5 Mn0.083 O0.333 F0.083
Na0.2 Li0.3 Ga0.1 O0.4
Li0.5 Fe0.083 O0.333 F0.083
Li0.489 Si0.051 P0.022 S0.365 I0.073
Li0.5 S0.5
K0.1 Li0.4 Al0.1 O0.4
Li0.5 S0.25 Br0.25
Li0.5 O0.2 Br0.3
Li0.5 Ga0.1 S0.4
Na0.5 O0.5
K0.05 Na0.45 In0.1 O0.4
Na0.5 Sn0.125 O0.375
Li0.5 Mn0.071 O0.214 F0.214
Li0.5 Al0.1 S0.4
Na0.25 Li0.25 S0.5
Li0.5 Se0.25 Cl0.25
Rb0.061 Li0.424 Pb0.091 O0.424
Rb0.2 Li0.3 Ga0.1 O0.4
Li0.485 Si0.044 P0.029 S0.368 I0.074
Li0.5 Mn0.1 O0.3 F0.1
Li0.5 Se0.5
Cs0.061 Li0.424 Pb0.091 O0.424
Li0.5 Te0.25 Cl0.25
K0.3 Na0.2 In0.1 O0.4
Na0.5 S0.25 I0.25
Li0.333 Eu0.167 O0.5
Ra0.5 S0.5
3.5
3
2.5
2
1.5
1
0.5
0

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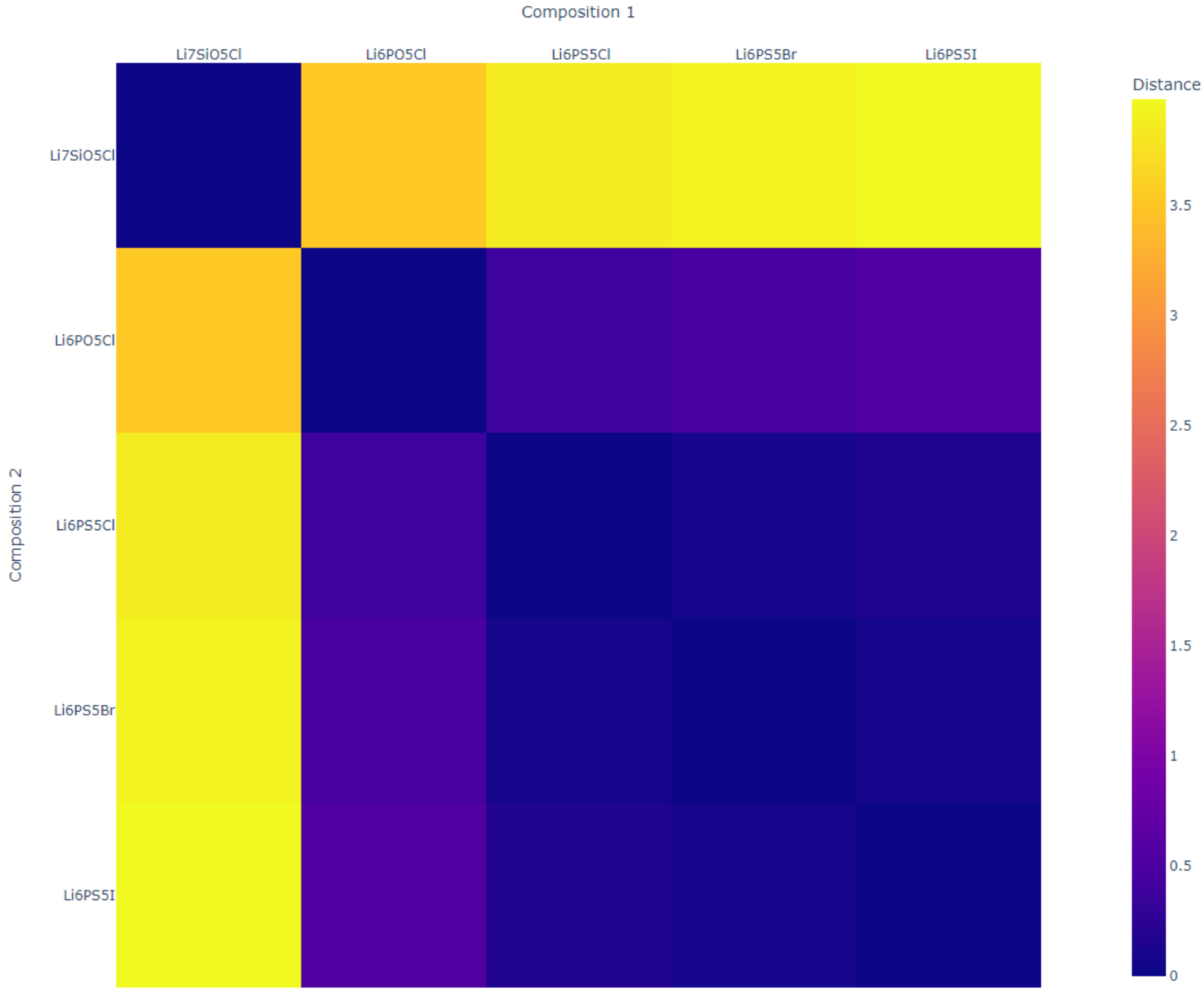
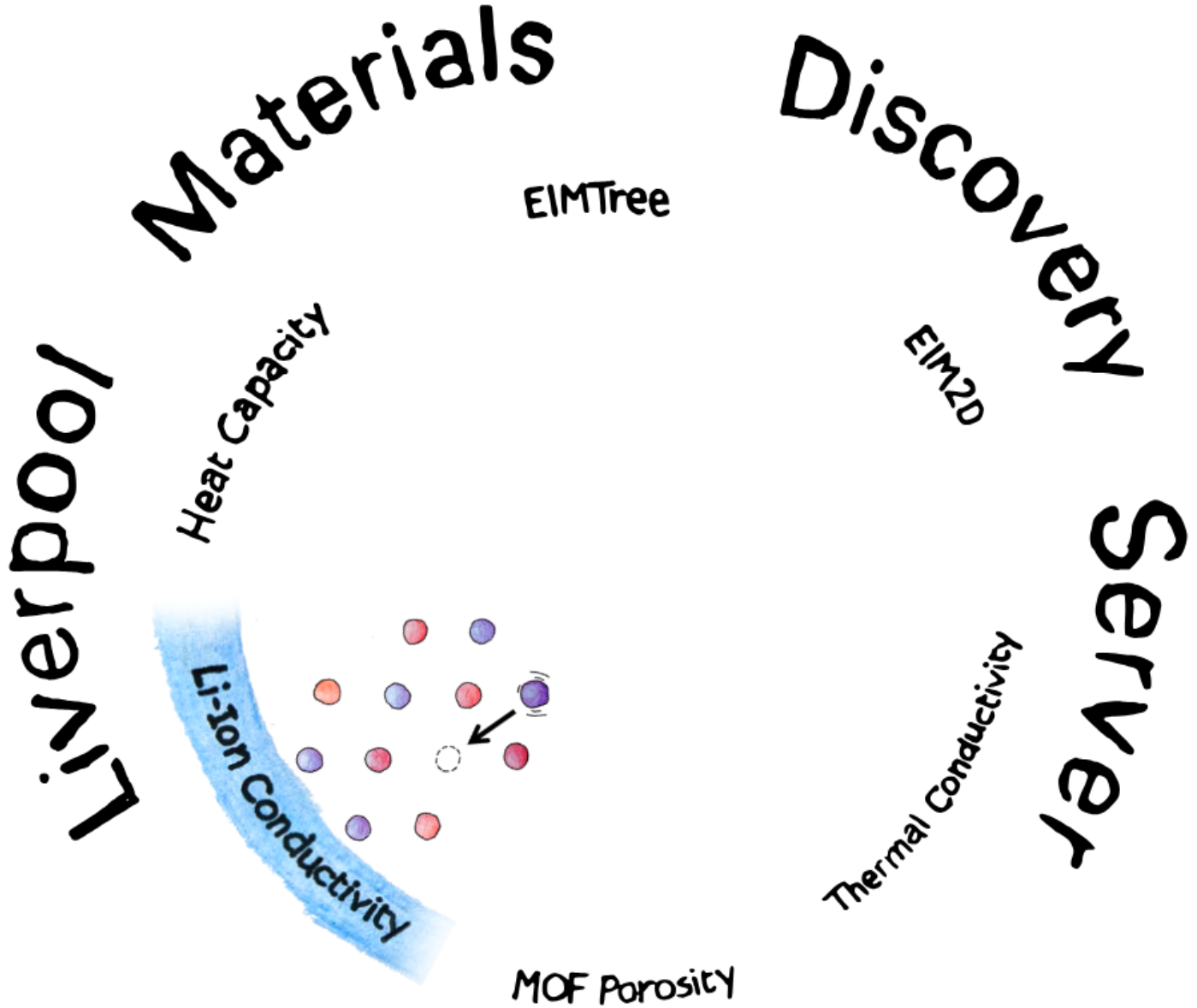
ElM2D

Li7SiO5Cl, Li6PO5Cl, Li6P

Enter a composition to see the 100 most similar ElMTree indexed compositions, embedded to two dimensions via UMAP. Enter up to 100 compositions, separated via commas, to plot their chemical similarity. Tap the distance matrix to view specific distances. This application was reported in The Liverpool Materials Discovery Server: A suite of tools for the collaborative discovery of materials, and implements the process described in The Earth Movers Distance as a Metric for the space of Inorganic Compositions. Please consider citing these papers if you use this in your work.


Composition 1
Li7SiO5Cl
Li6PO5Cl
Li6PS5Cl
Li6PS5Br
Li6PS5I
Composition 2
Li7SiO5Cl
Li6PO5Cl
Li6PS5Cl
Li6PS5Br
Li6PS5I
Distance
3.5
3
2.5
2
1.5
1
0.5
0



Predict the ionic conductivity of potential formulations for solid state electrolytes from the composition

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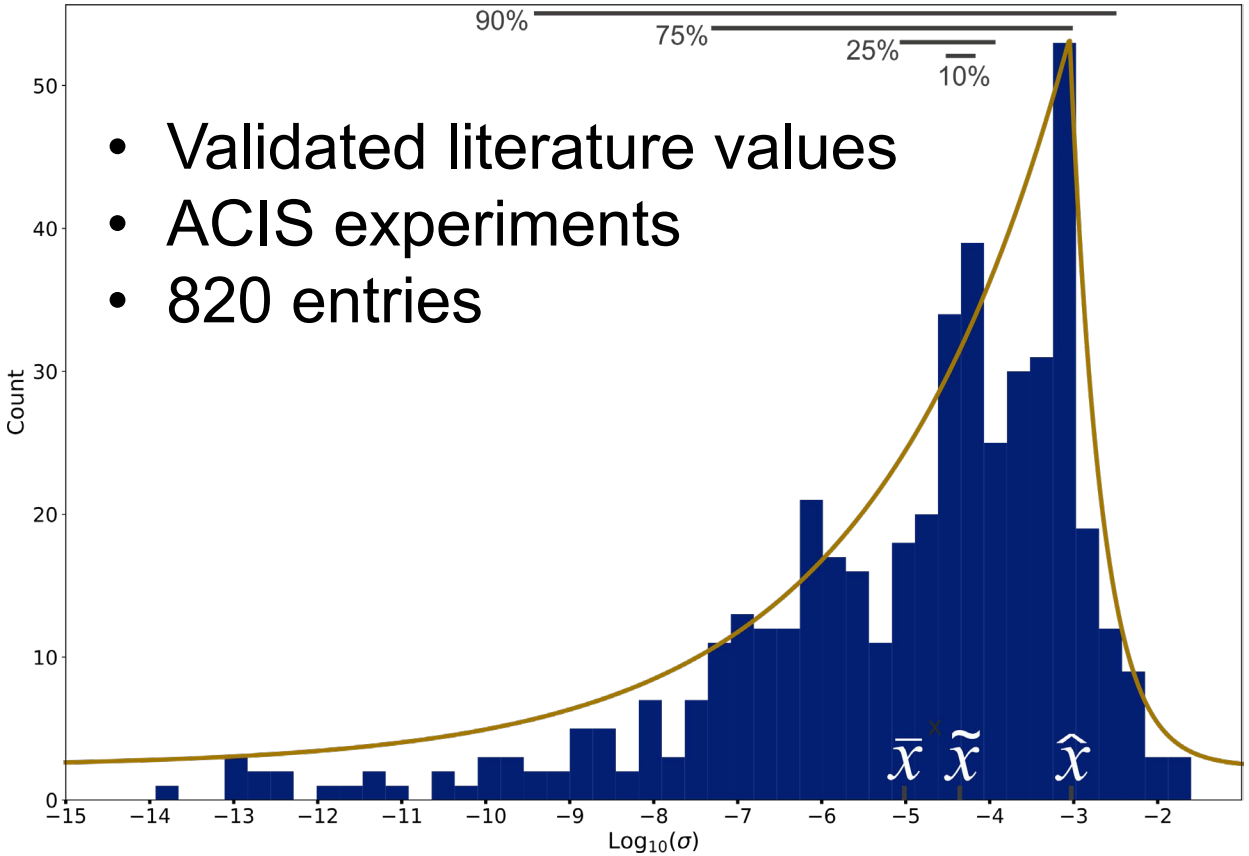
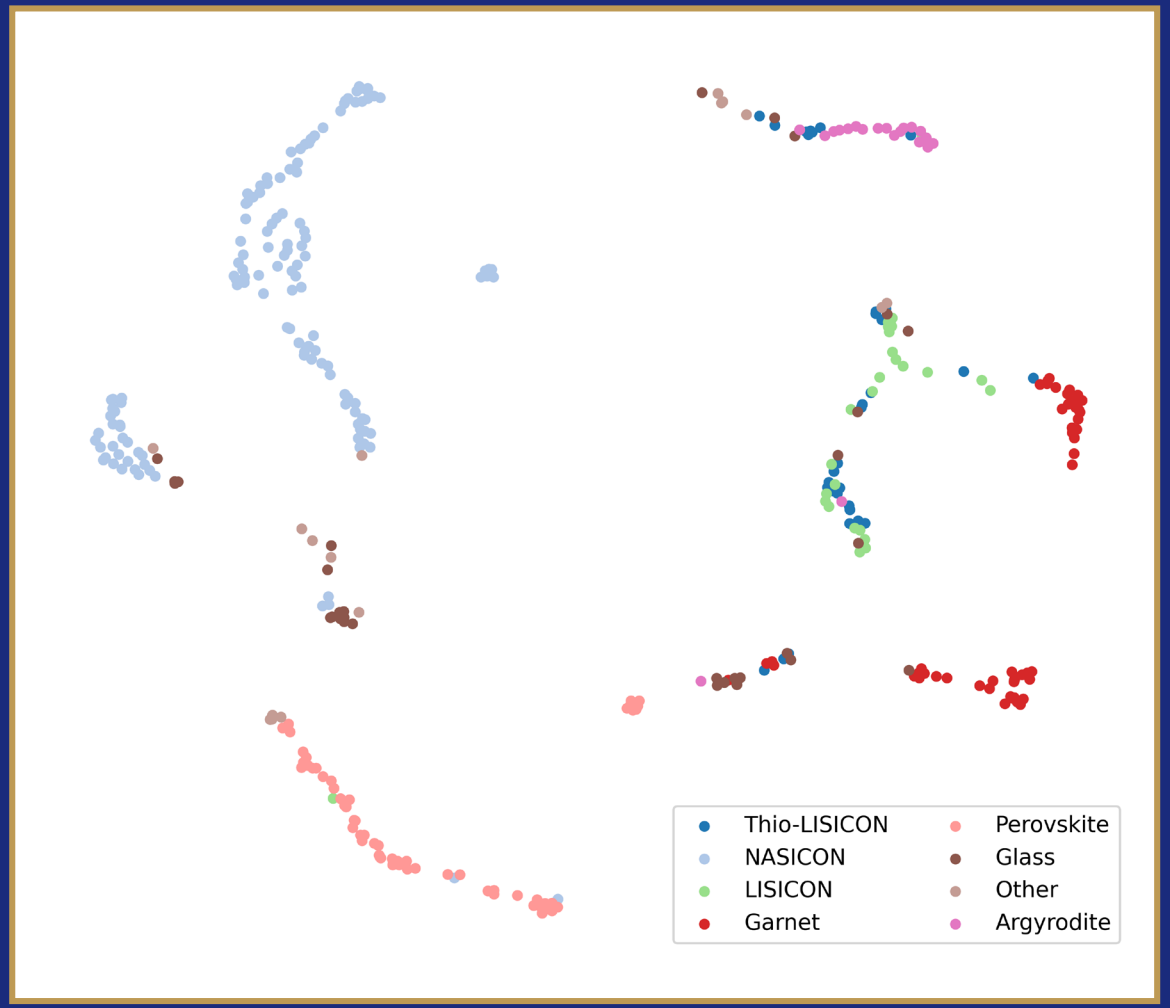
Li Ion Conductivity Background



http://pcwww.liv.ac.uk/~msd30/lmds/LiIonDatabase.html



C J Hargreaves, et al. *npj Comput. Mater.* **9** (2023) 9

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Liverpool Materials Discovery Server LMDS

Li-Ionic Conductivity

Li7SiO5Cl, Li6PO5Cl, Li6PS5Cl, Li6PS5Br, Li6PS5I

Calculate

Enter the chemical composition (or a list of up to 2,000 compositions separated by commas) of a candidate Li conducting solid state electrolyte to return a binary classification prediction of whether a material will have a conductivity > 10^{-4} S cm^{-1}, and a regression prediction of the materials conductivity in $\log_{10}$(S cm^{-1}). These classification predictions were found to have an accuracy of 0.71, with regression predictions having a mean absolute error of 0.99. This is based on a CrabNet architecture, trained on The Liverpool Ionics Dataset, and is a hosted version of the deep learning model introduced in A database of experimentally measured lithium solid electrolyte conductivities evaluated with machine learning and reported in The Liverpool MaterialS Discover server: A Suite of Computational Tools for the Collaborative discovery of Materials. Please consider citing these papers if you use this tool in your work.

If you would like to access this tool via API click here for more information

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Liverpool Materials Discovery Server LMDS

Li-Ionic Conductivity

Li7SiO5Cl, Li6PO5Cl, Li6PS5Cl, Li6PS5Br, Li6PS5I

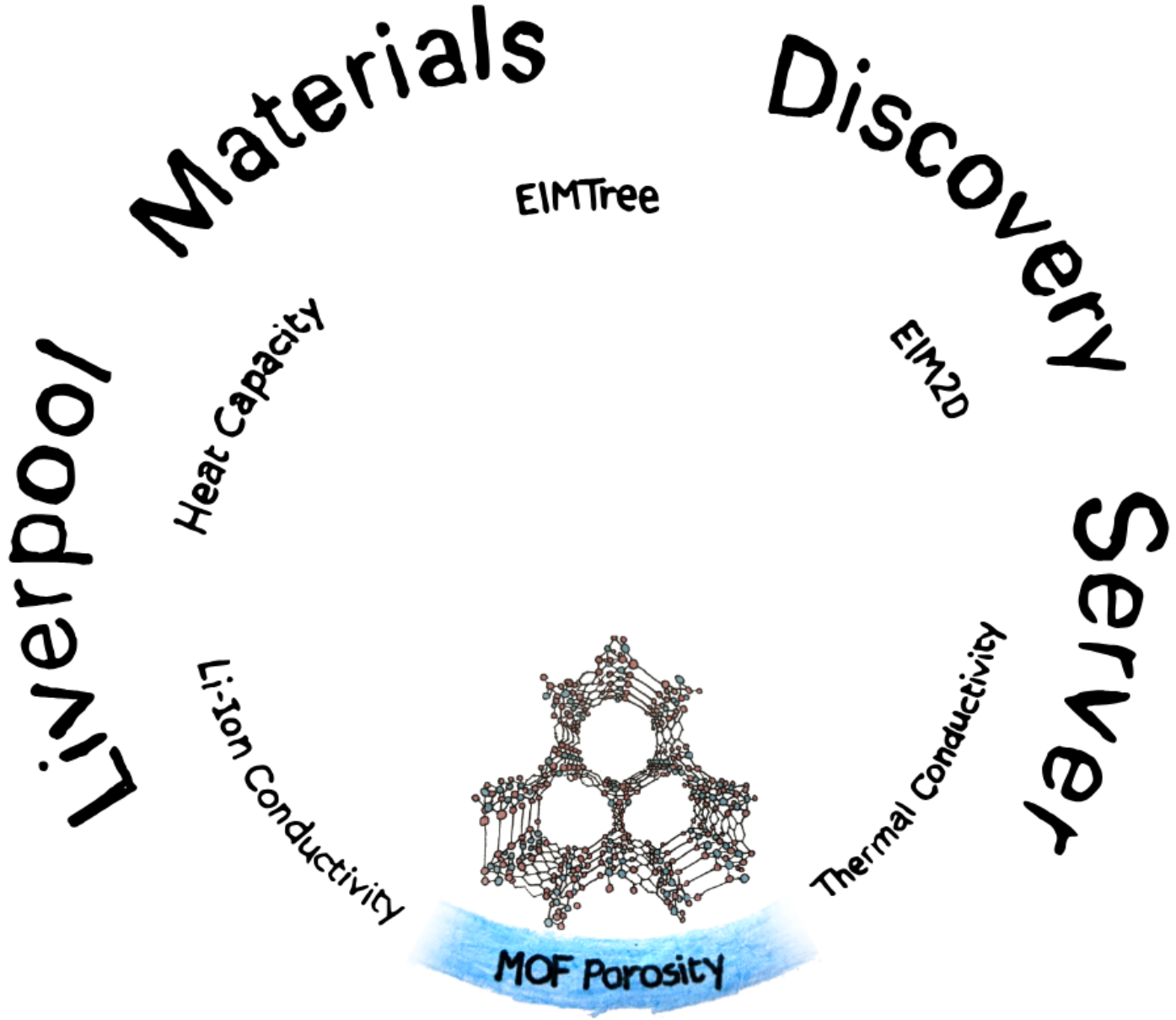
Calculate

Composition	Classification Model (> 10^{-4})	Regression Model ($log_{10}(Scm^{-1})$)
Li7SiO5Cl	0	-8.43
Li6PO5Cl	0	-9.36
Li6PS5Cl	1	-3.25
Li6PS5Br	1	-3.11
Li6PS5I	1	-3.15

Download as csv

Accuracy ~ 81 %

MAE on log_{10}(conductivity) = 0.85



Predict whether a MOF is likely to be porous using the SMILES representation of the linker and a chosen metal

Rémi Pétuya

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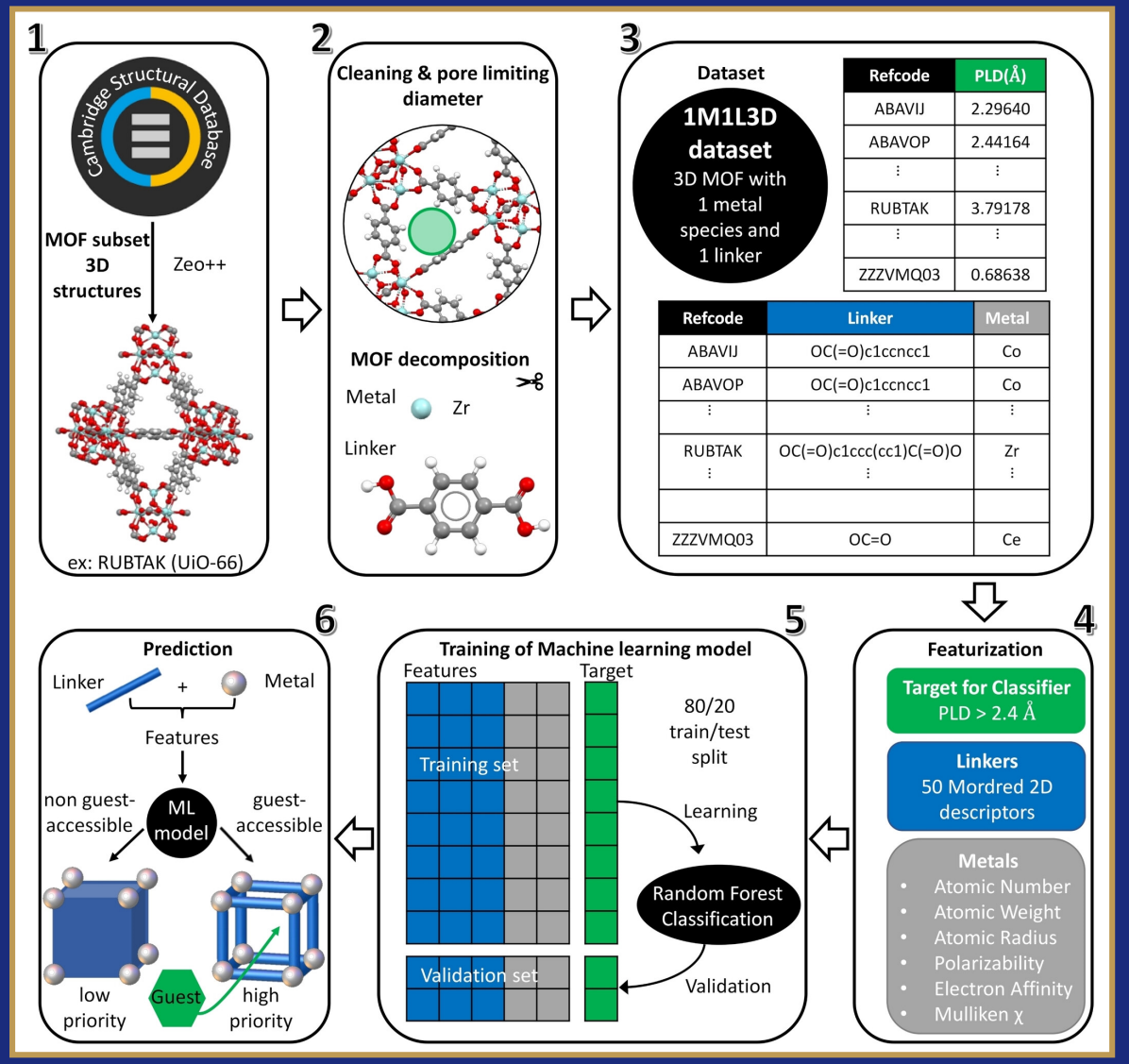
MOF Porosity Background

- Metal organic frameworks are porous materials with inorganic and organic fragments
- Experimentally determined structures are reported in the CSD
- We took these and split them into separate metal / organic fragments to enable machine learning prediction of porosity



R Pétuya, *et al*. *Angew. Chem. Int. Ed.* (2022) e202114573

Rémi Pétuya

MOF Porosity

OC(=O)C(=O)O

Zr, Zn, Cu, Fe

Calculate

Enter the formulation of a potential MOF using the SMILES representation of the linker and the metal(s) to be combined, to predict the likelihood of pores of different sizes forming in the resultant structur. Due to limitations in the training dataset only some elements are supported as metal, find the list of elements supported here. Predictions were found to have an accuracy of 80.5% on a test set. This application was reported in The Liverpool Materials Discovery Server: A suite of tools for the collaborative discovery of materials. and is based on the model first reported in Machine-Learning Prediction of Metal–Organic Framework Guest Accessibility from Linker and Metal Chemistry. Please consider citing these papers if you use this in your work.

Click here for information about accessing this model using our API

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Liverpool Materials Discovery Server LMDS

Rémi Pétuya

MOF Porosity

OC(=O)C(=O)O

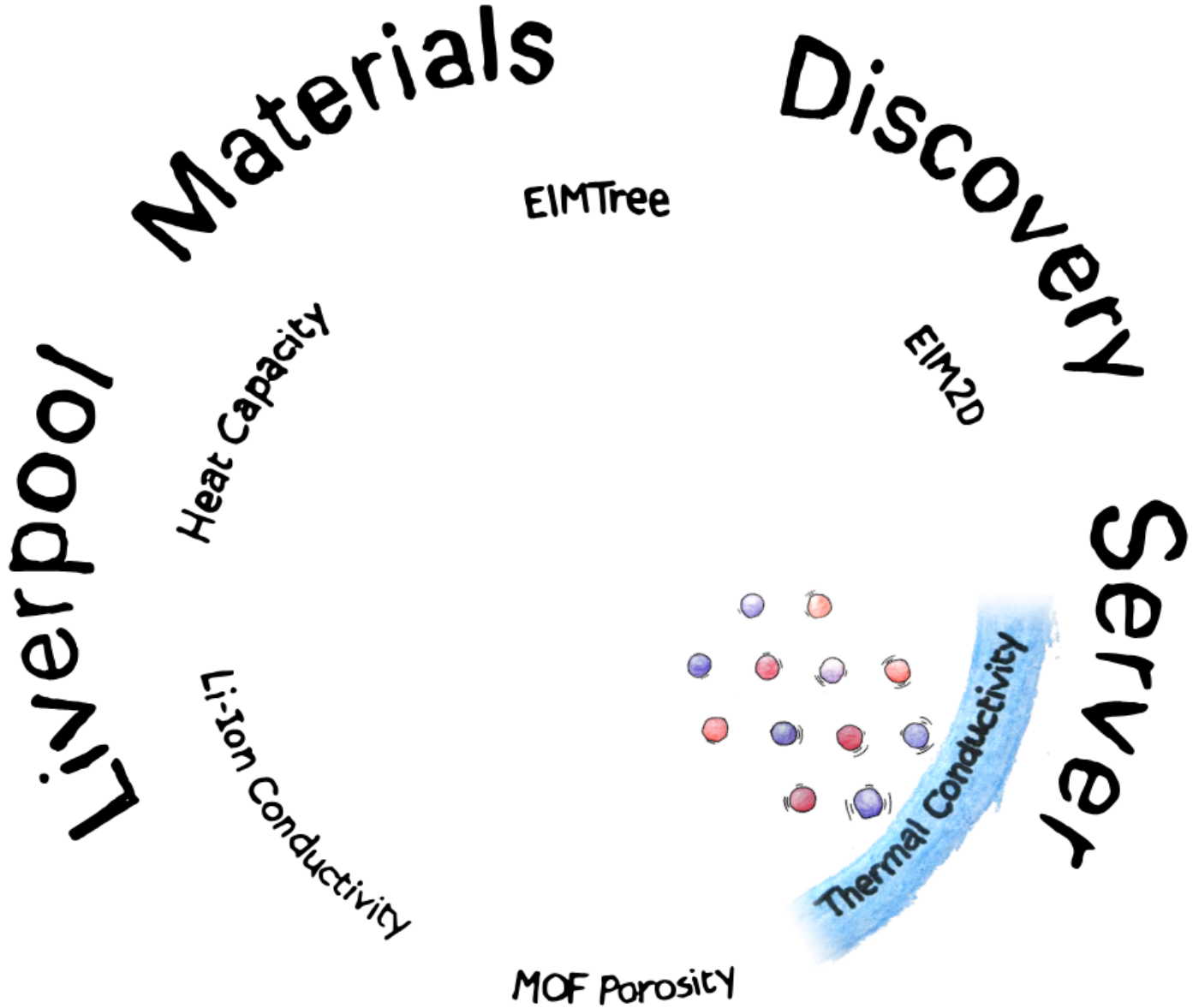
Zr, Zn, Cu, Fe

Calculate

Download as csv

Linker	Metal	Predicted porosity category
OC(=O)C(=O)O	Zr	porosity < 2.4 Å
OC(=O)C(=O)O	Zn	2.4Å < porosity < 4.4Å
OC(=O)C(=O)O	Cu	4.4Å < porosity <5.9Å
OC(=O)C(=O)O	Fe	2.4Å < porosity < 4.4Å

Accuracy ~ 80 %



Predict the thermal conductivity of a candidate thermoelectric material from its composition

Michael Moran

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Liverpool Materials Discovery Server LMDS

Thermal Conductivity

Cu9Al4, Sr2Ti6O13, Ti2FeNiSb2, Cu2SnZnS4

Calculate

Enter a composition, or a list of up to 2000 compositions separated by commas, to return a prediction of the thermal conductivity of each formulation.The prediction was found to have a R^2 of 0.71, and root mean squared error of 0.55 $\log_{10}(W\ m^{-1}\ K^{-1})$ on a test set of thermoelectric materials comparing the true logarithm of thermal conductivity to the predicted logarithm of thermal conductivity. This application was reported in The Liverpool Materials Discovery Server: A suite of tools for the collaborative discovery of materials., and is an improved version of the model first used in Discovery of a Low Thermal Conductivity Oxide Guided by Probe Structure Prediction and Machine Learning. Please consider citing these papers if you use this in your work.

Click here for information as to how to use this model with an API

Michael Moran

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Liverpool Materials Discovery Server LMDS

Thermal Conductivity

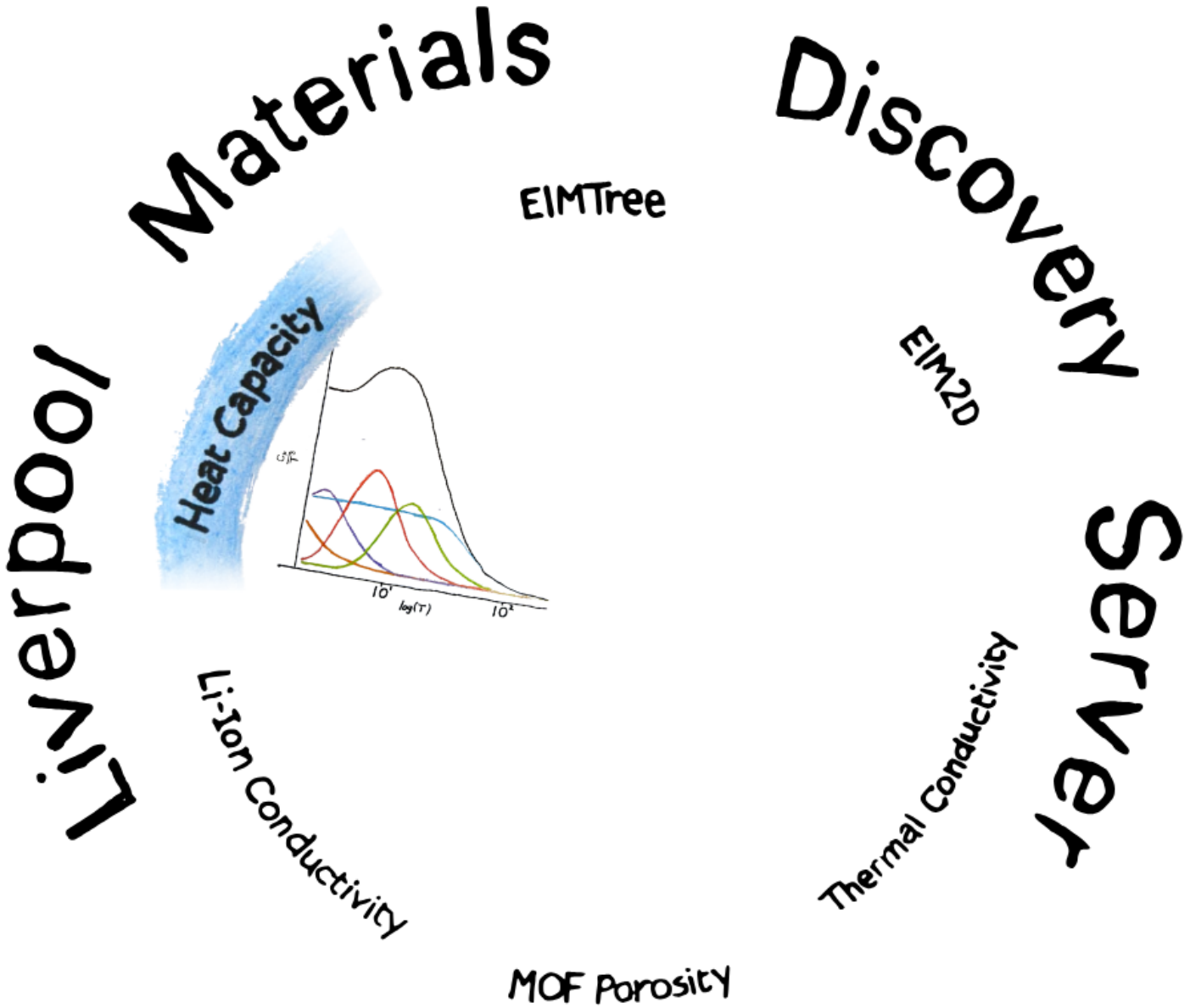
Cu9Al4, Sr2Ti6O13, Ti2FeNiSb2, Cu2SnZnS4

Calculate

Download as csv

Composition	Predicted thermal conductivity (W m^{-1} K^{-1})
Cu9Al4	15.78
Sr2Ti6O13	9.91
Ti2FeNiSb2	6.19
Cu2SnZnS4	7.5

RMSE on $\log_{10}$(conductivity) = 0.55



Model the heat capacity of a material from a csv of temperature readings and the corresponding Einstein and Debye components

Heat Capacity

Jon Newnham

Choose File ExampleData.csv

Einstein components

Add Einstein component | Remove Einstein component

Debye Components

Debye Temperature 1 (K)

300

Pre-factor component for 1

1

Add Debye component | Remove Debye component

Linear (γ) component

0

Plot data as C_p/T^n (n = 0 for high T fitting, 3 for low T fitting)

0

Model Starting Temperature (K)

2

Model Ending Temperature (K)

250

X axis log scale? ☐

Y axis log scale? ☐

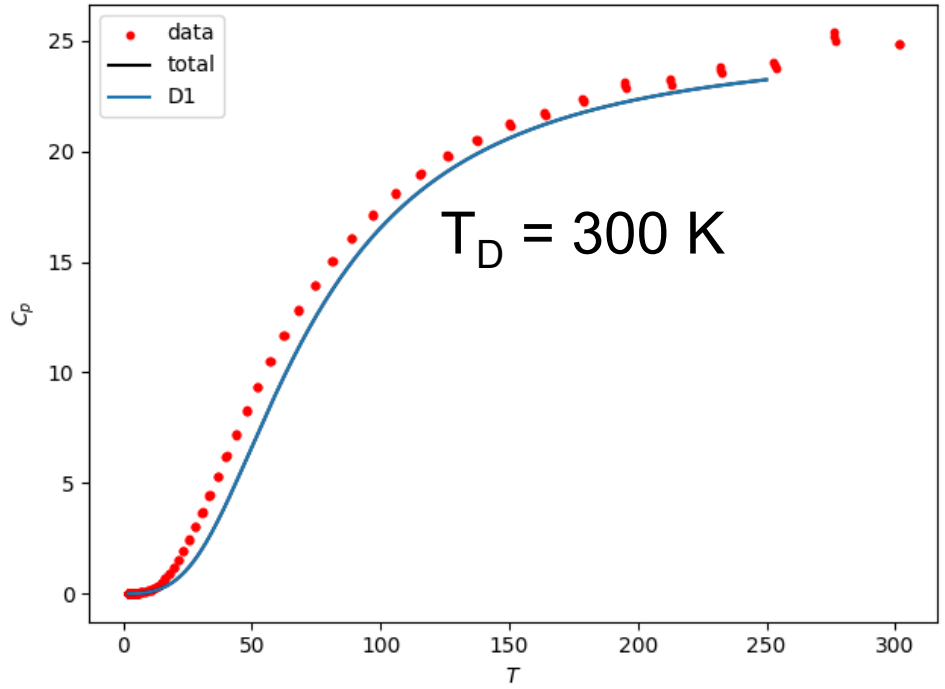
Calculate

Jon Newnham

Heat Capacity

Choose File No file chosen

Your file is already uploaded and will be stored for 15 minutes, there is no need to reupload file unless wish to change the data you are operating on



Click here to download your model

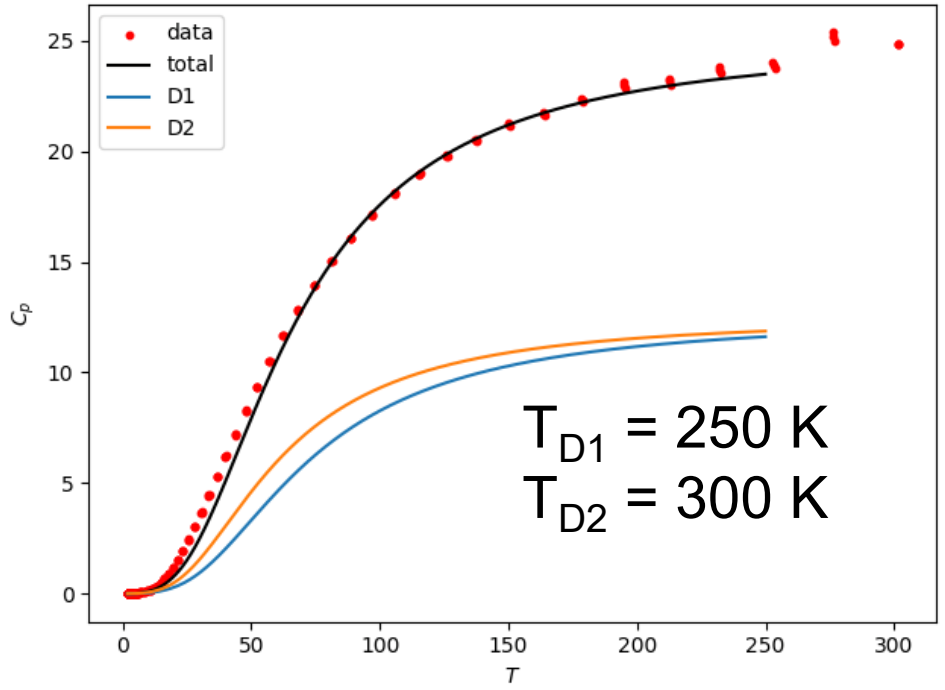
Einstein components

Jon Newnham

Heat Capacity

Choose File No file chosen

Your file is already uploaded and will be stored for 15 minutes, there is no need to reupload file unless wish to change the data you are operating on



Click here to download your model

Einstein components

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Conclusions

- The LMDS is up and running, and freely available to all
- Cloud based web-servers like the LMDS are a good way to make computational models available for wide use
- The LMDS server will be expanded in the future, so watch this space!

https://lmds.liverpool.ac.uk

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Acknowledgements

- Sam Durdy
- Cameron Hargreaves
- Matt J Rosseinsky
- Michael W Gaultois
- Michael Moran
- Jon A Newnham
- Rémi Pétuya
- Mark Dennisson
- Benjamin Wagg

Ramsay Trust Memorial Fellowship

EPSRC Pioneering research and skills

THE FARADAY INSTITUTION

LEVERHULME TRUST

CloudPloys


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