HoW exciting 2023

Data analysis and quality assessment by fingerprinting

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HU BERLIN & IRIS ADLERSHOF

06.08.2023

Introduction

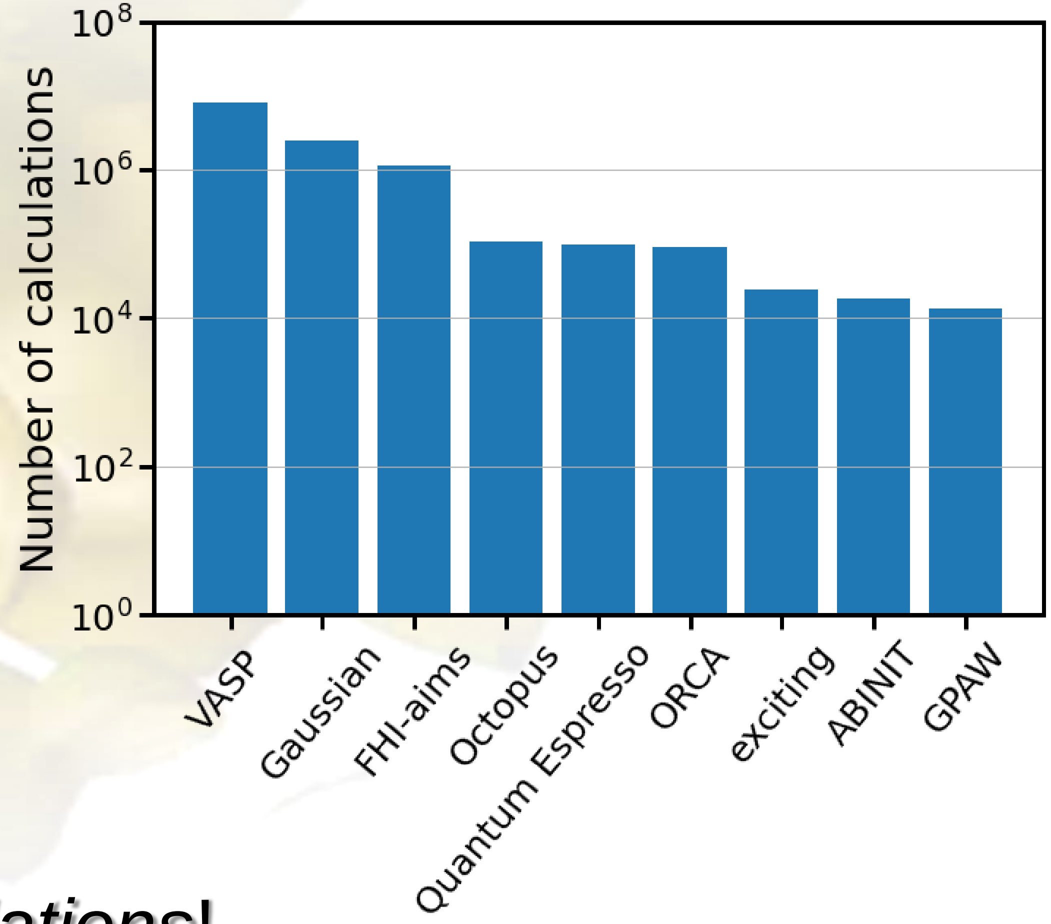
NOMAD Repository:

> 100 million calculations

> 40 codes

Interoperability?

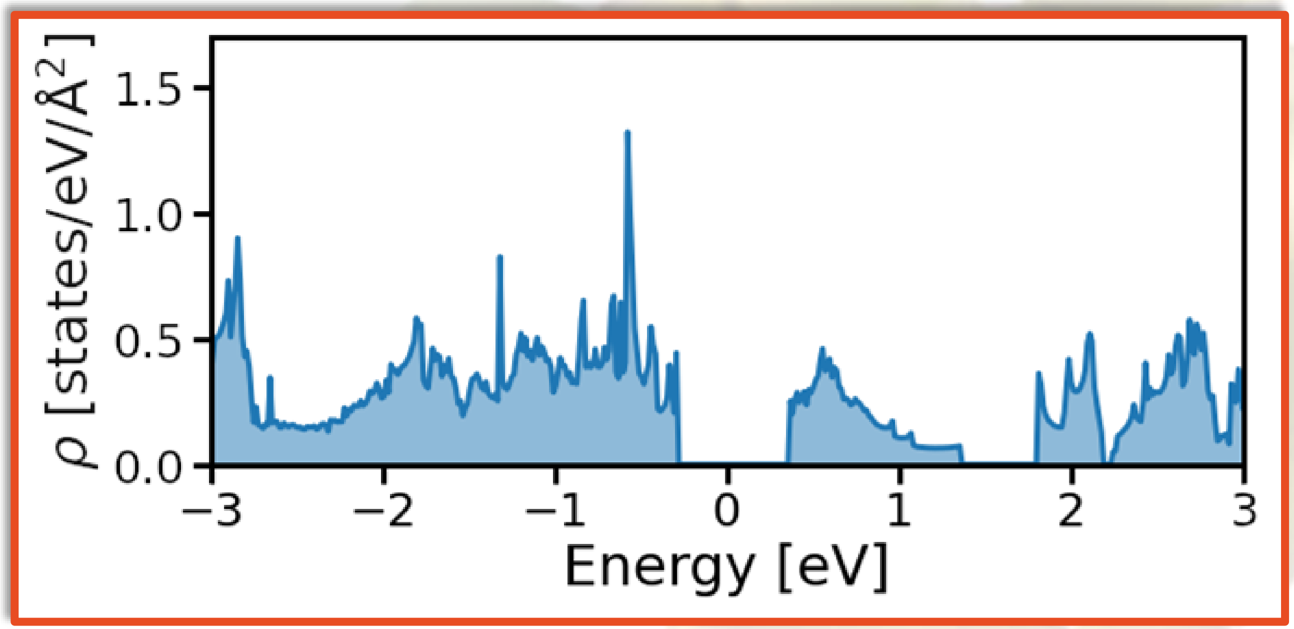
Findability?



09.10.2021

Analyze data using *similarity relations*!

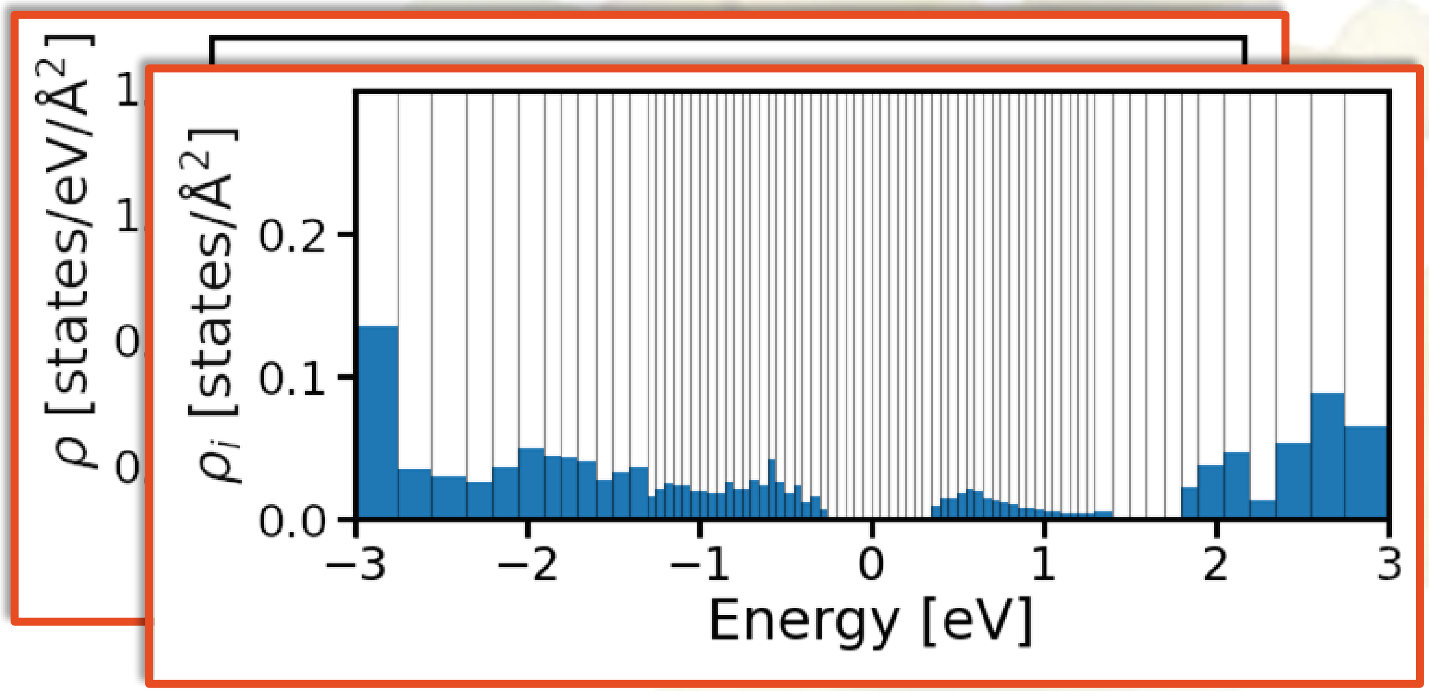
Spectrum fingerprints



M. Kuban *et al. Sci Data* **9**, 646 (2022).

Inspired by O. Isayev, et al., Chem. Mater. 27, 735 (2015)

Spectrum fingerprints



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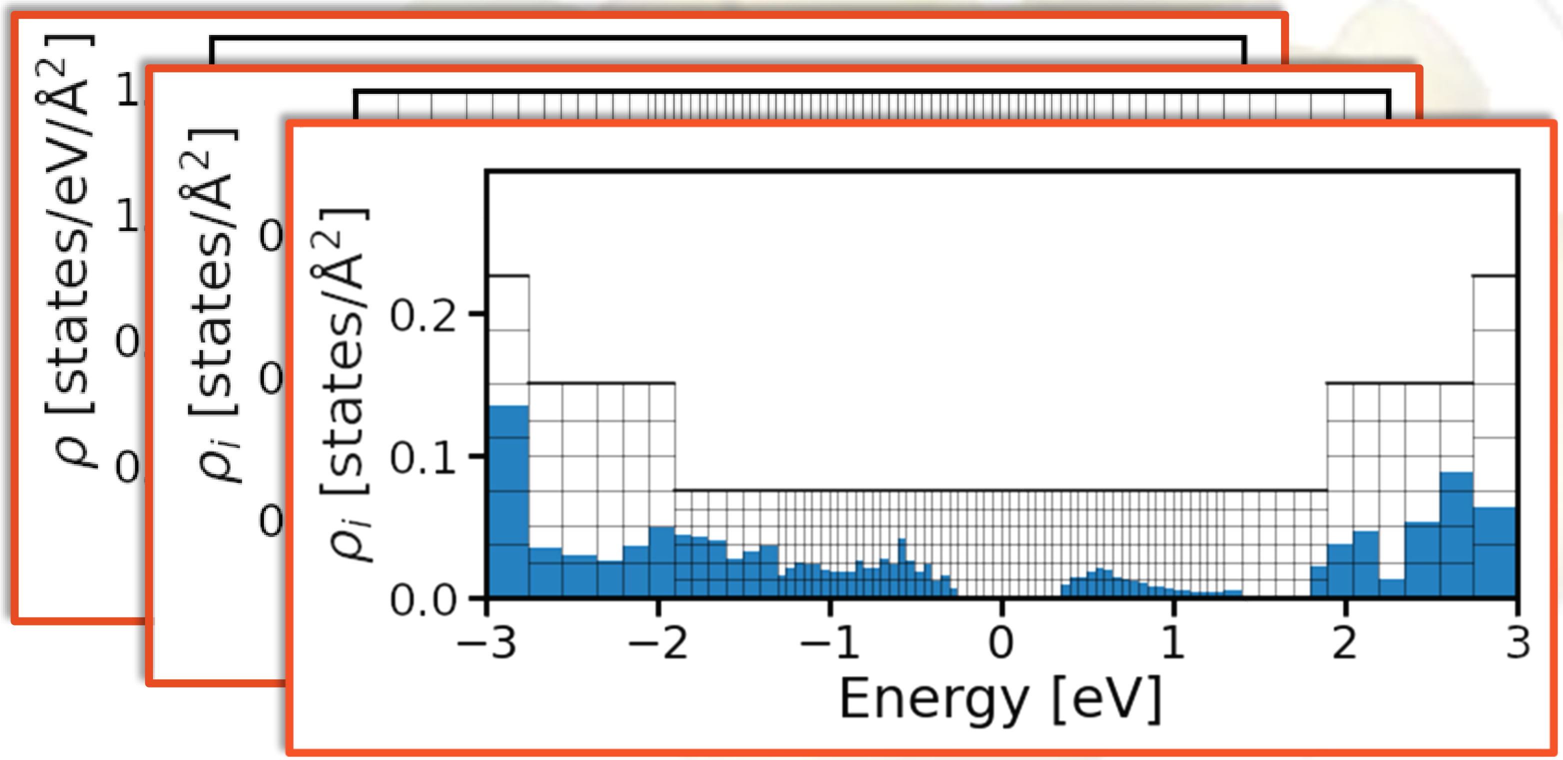
Spectrum fingerprints



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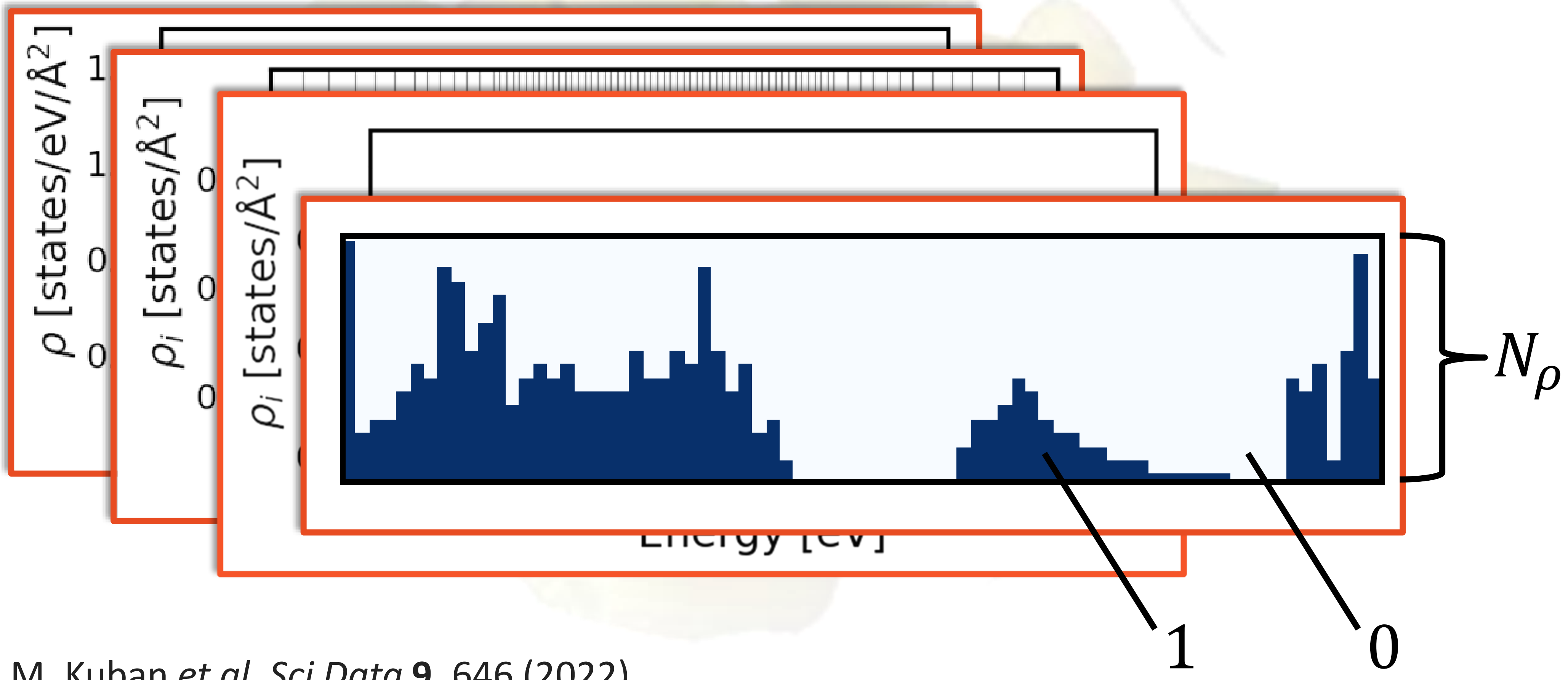
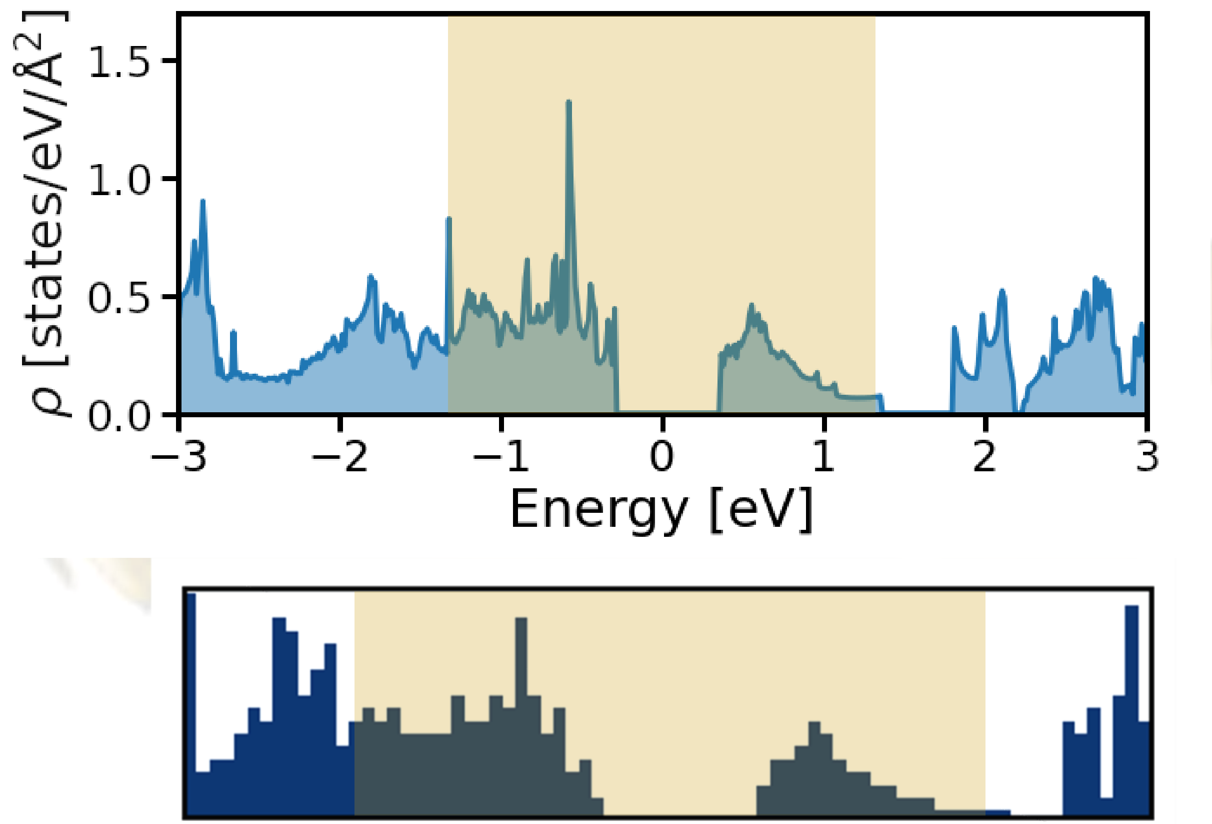
Spectrum fingerprints



M. Kuban *et al. Sci Data* **9**, 646 (2022).

Inspired by O. Isayev, et al., Chem. Mater. 27, 735 (2015)

Fingerprint feature region



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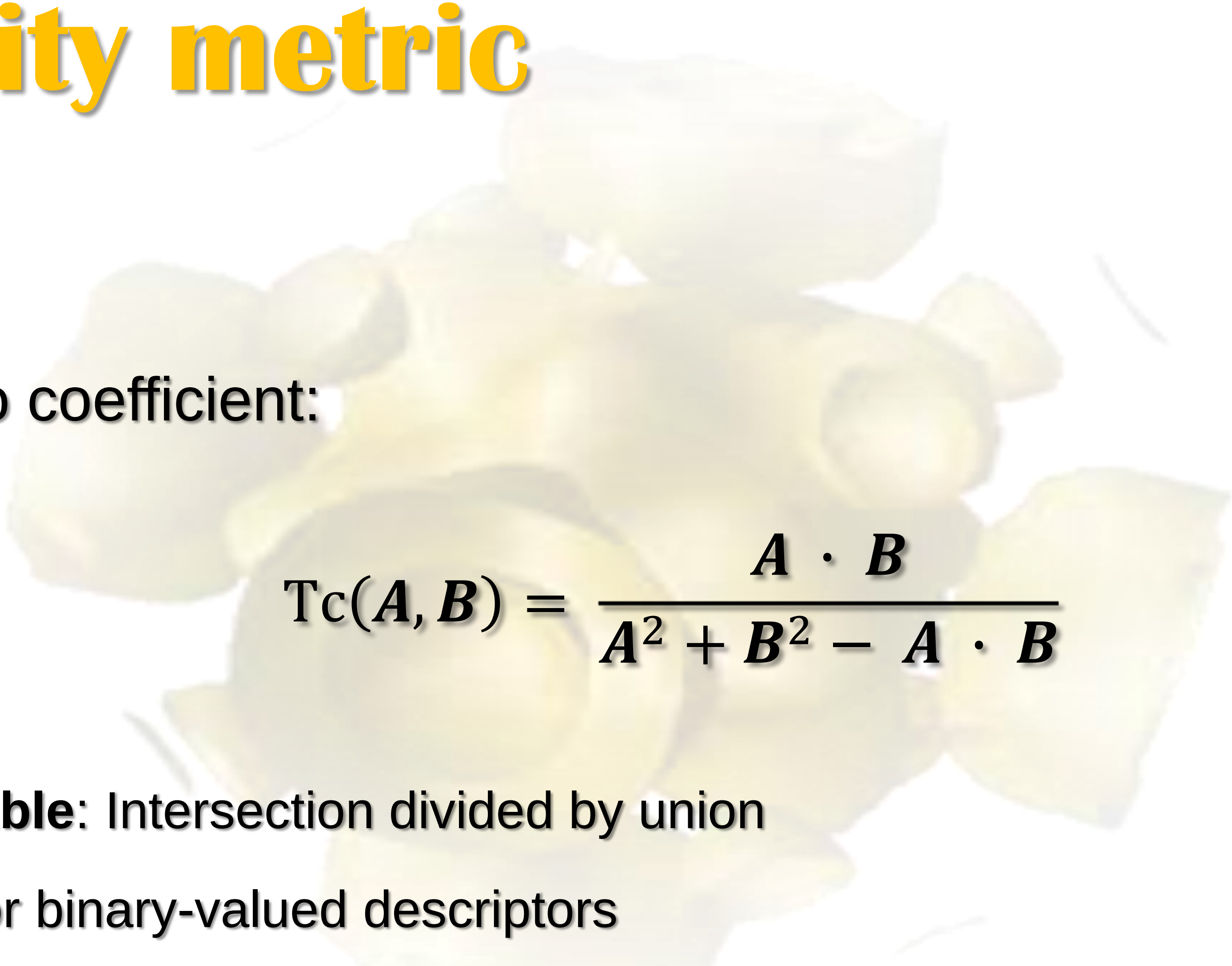
Similarity metric



Tanimoto coefficient:

$$\mathrm{Tc}(\boldsymbol{A},\boldsymbol{B}) = \frac{\boldsymbol{A}\cdot\boldsymbol{B}}{\boldsymbol{A}^2+\boldsymbol{B}^2-\boldsymbol{A}\cdot\boldsymbol{B}}$$

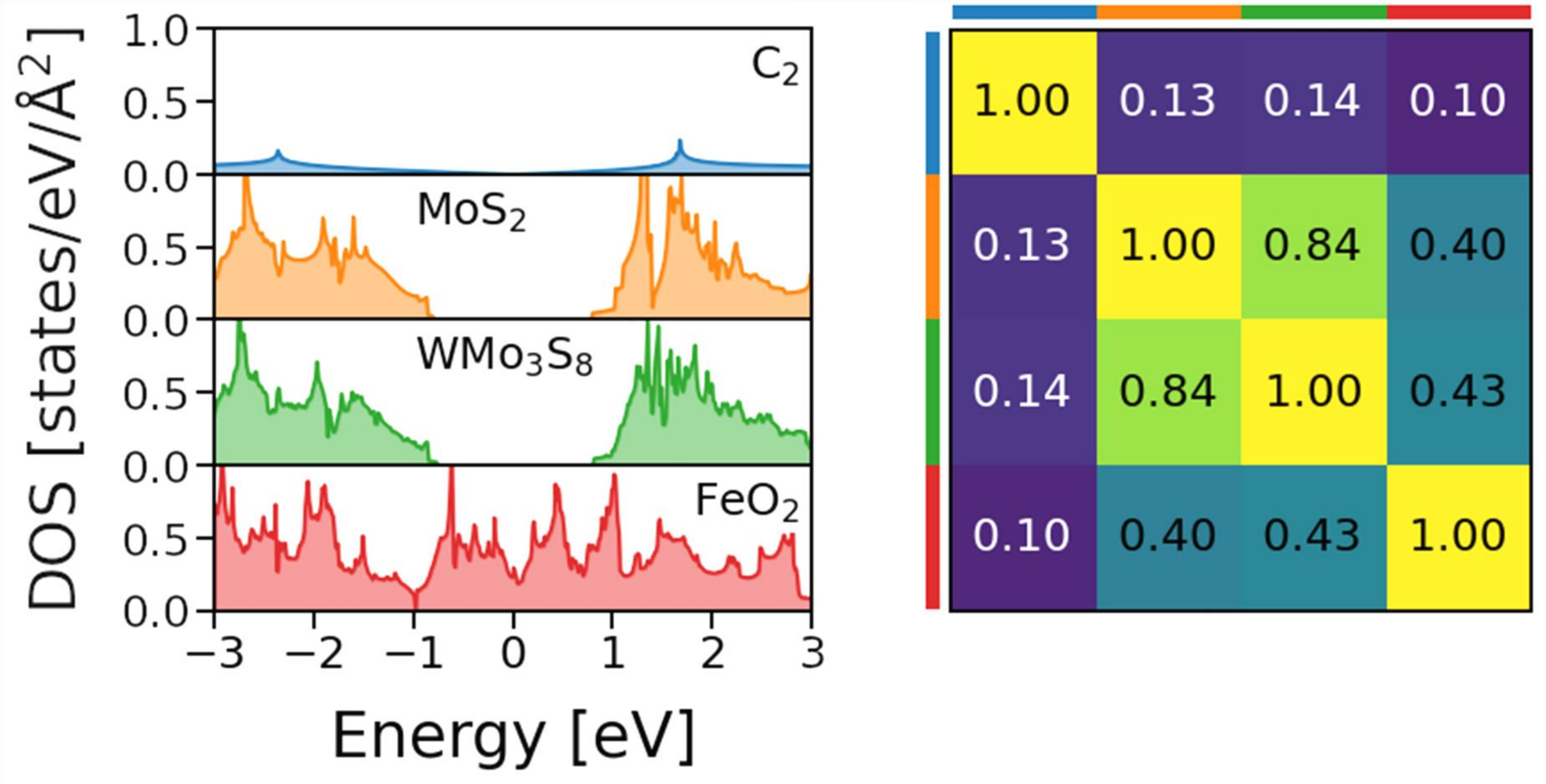
Interpretable: Intersection divided by union

Metric: For binary-valued descriptors

Computationally cheap: Can be described by bitwise operations

Peter Willet et al., *J. Chem. Inf. Comput. Sci.* **38**, 983–996 (1998)

Similarity metric



	🟦	🟧	🟩	🟥
🟦	1.00	0.13	0.14	0.10
🟧	0.13	1.00	0.84	0.40
🟩	0.14	0.84	1.00	0.43
🟥	0.10	0.40	0.43	1.00

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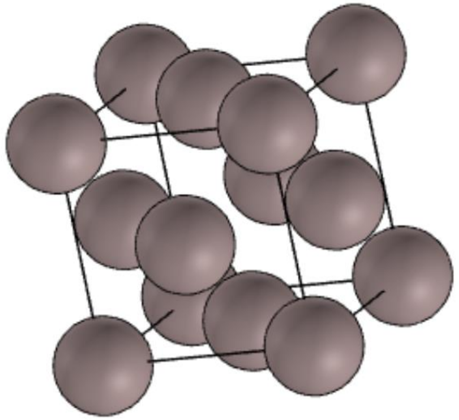
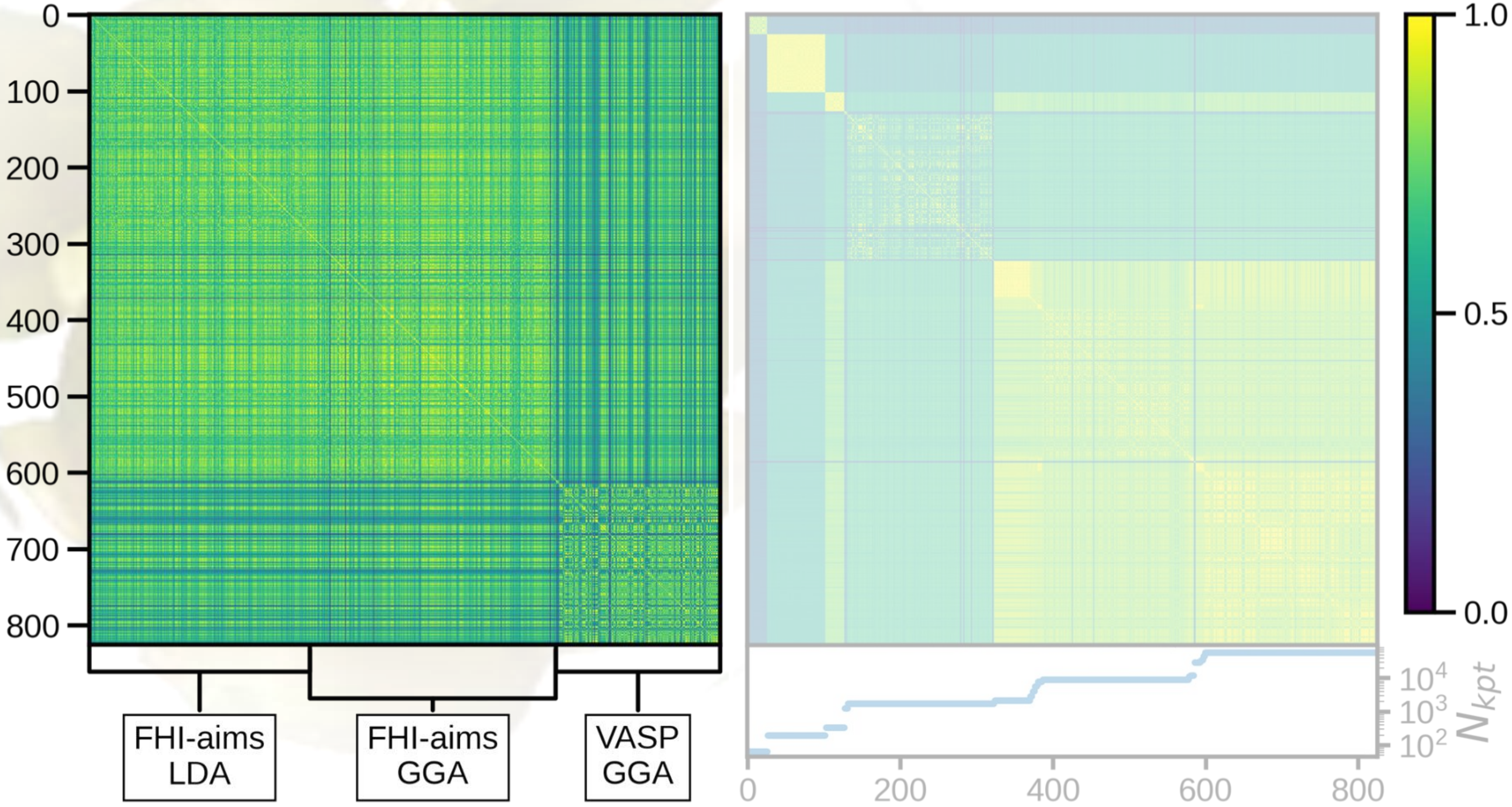
Data quality assessment

Code and computational parameters

NOMAD

fcc Al





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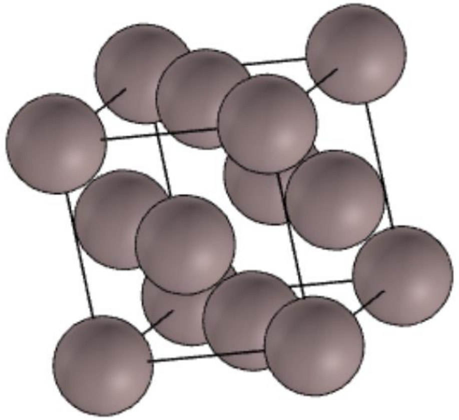

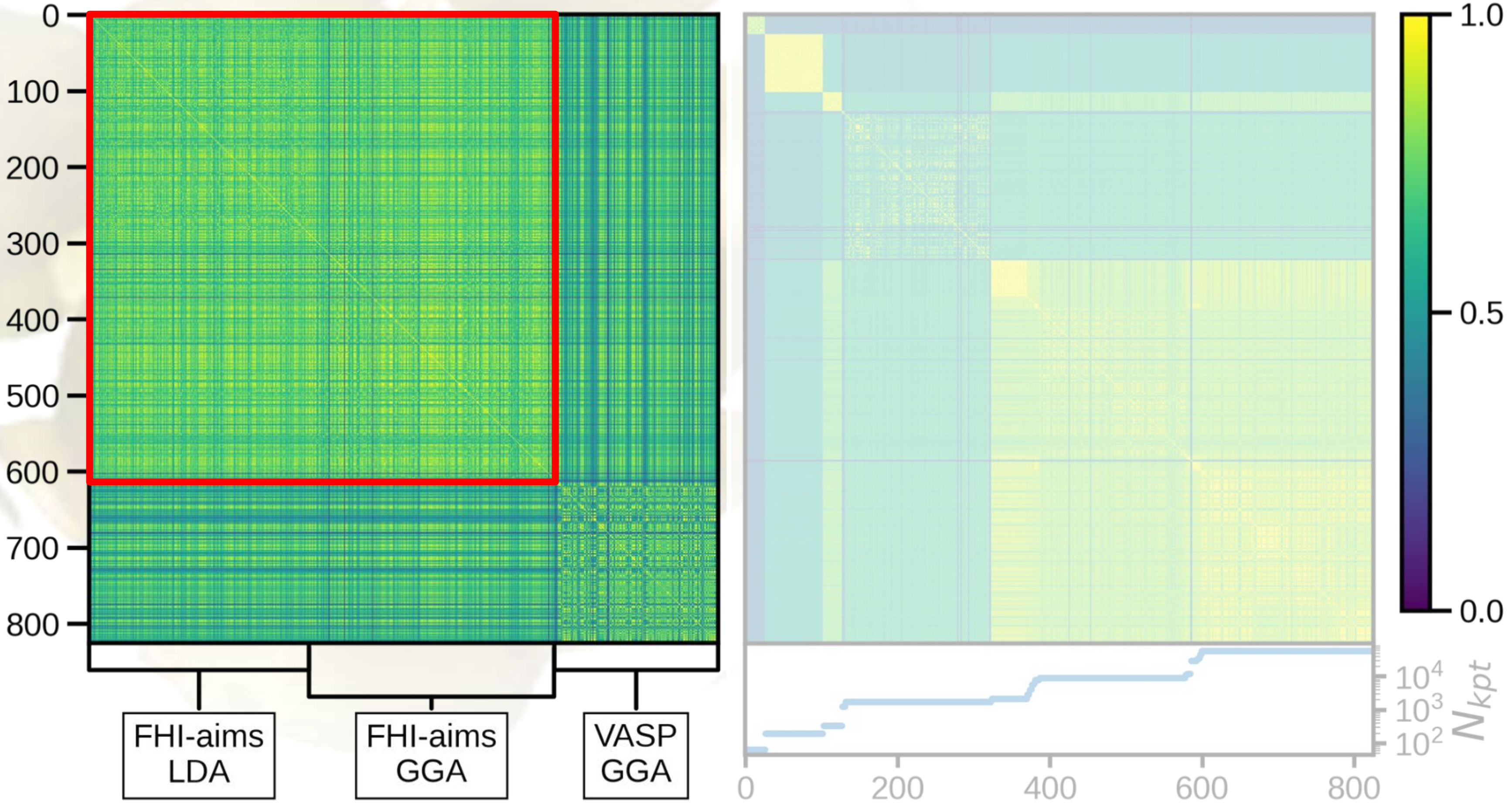

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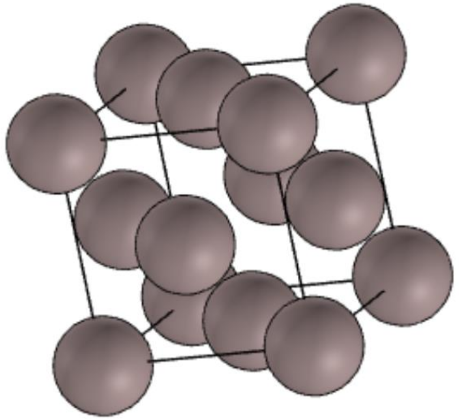

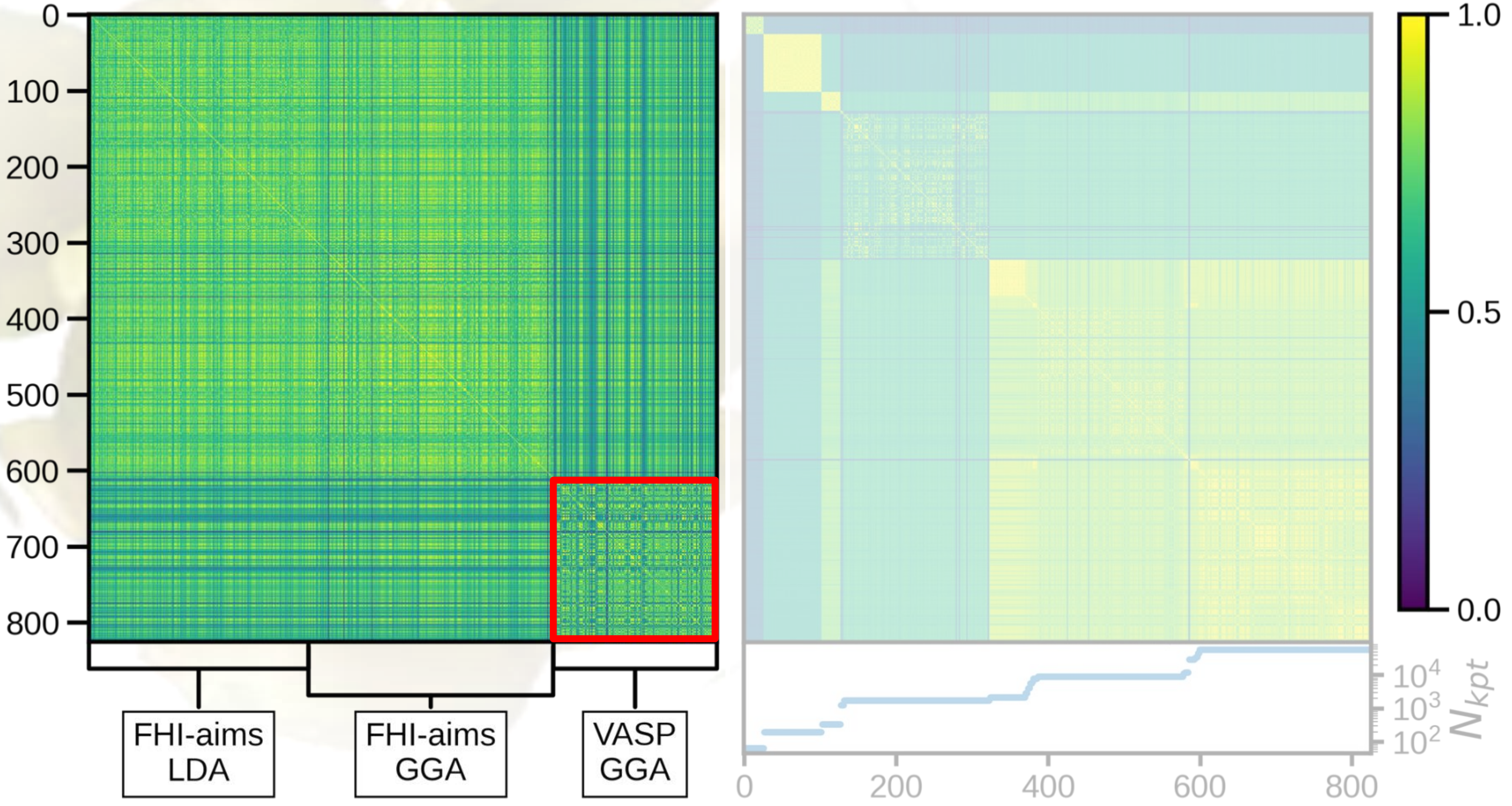

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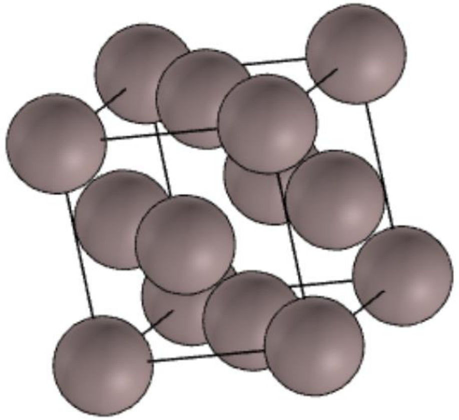

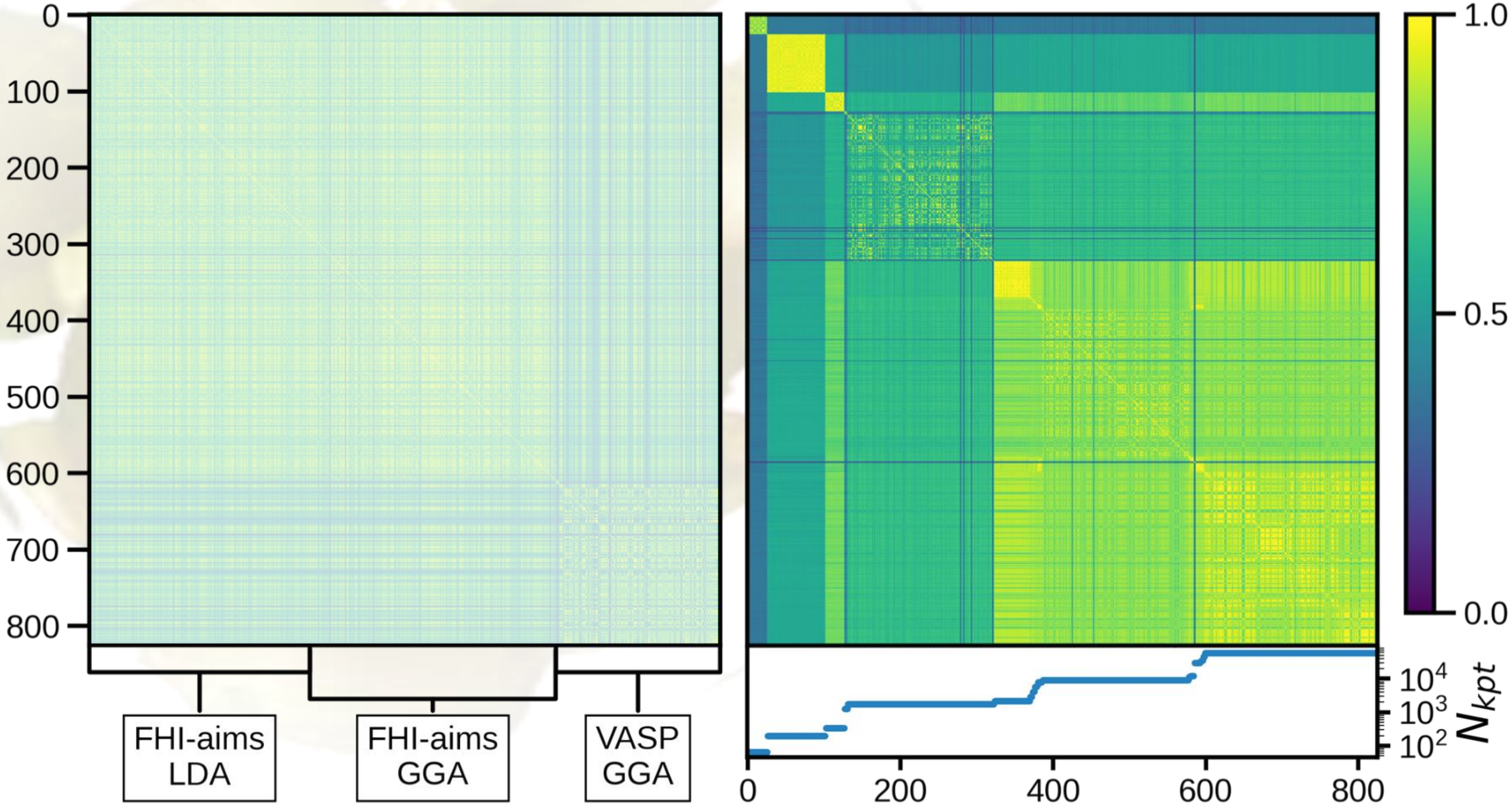

M. Kuban *et al.* MRS Bulletin **47**, 991–999 (2022).

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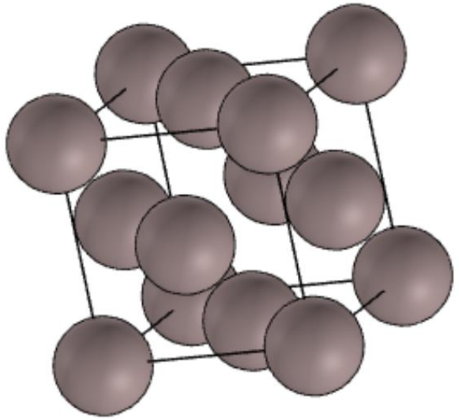

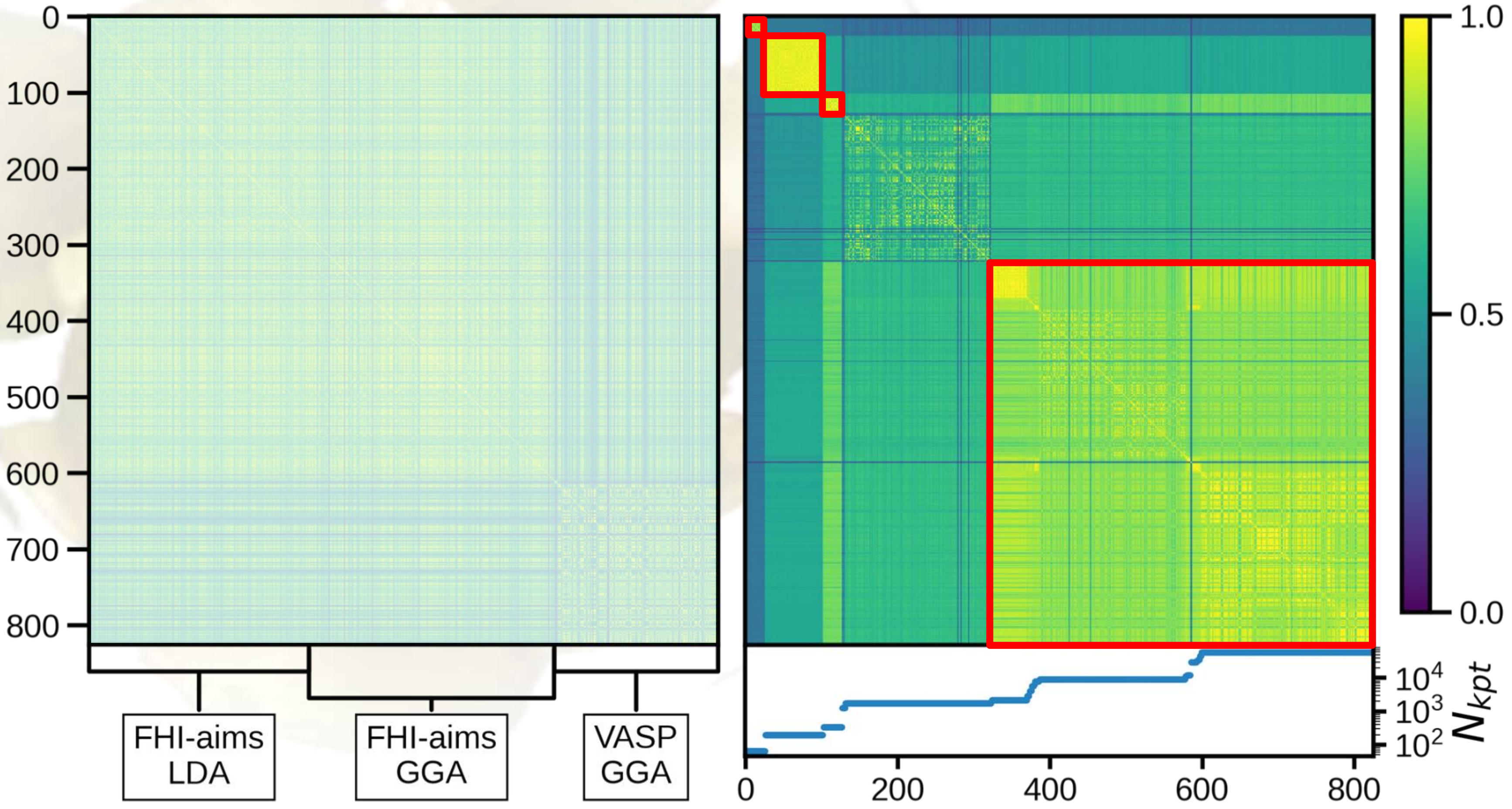

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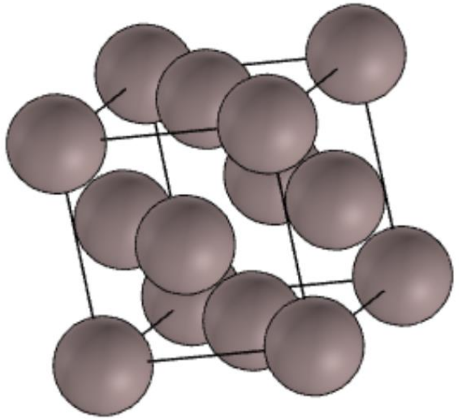

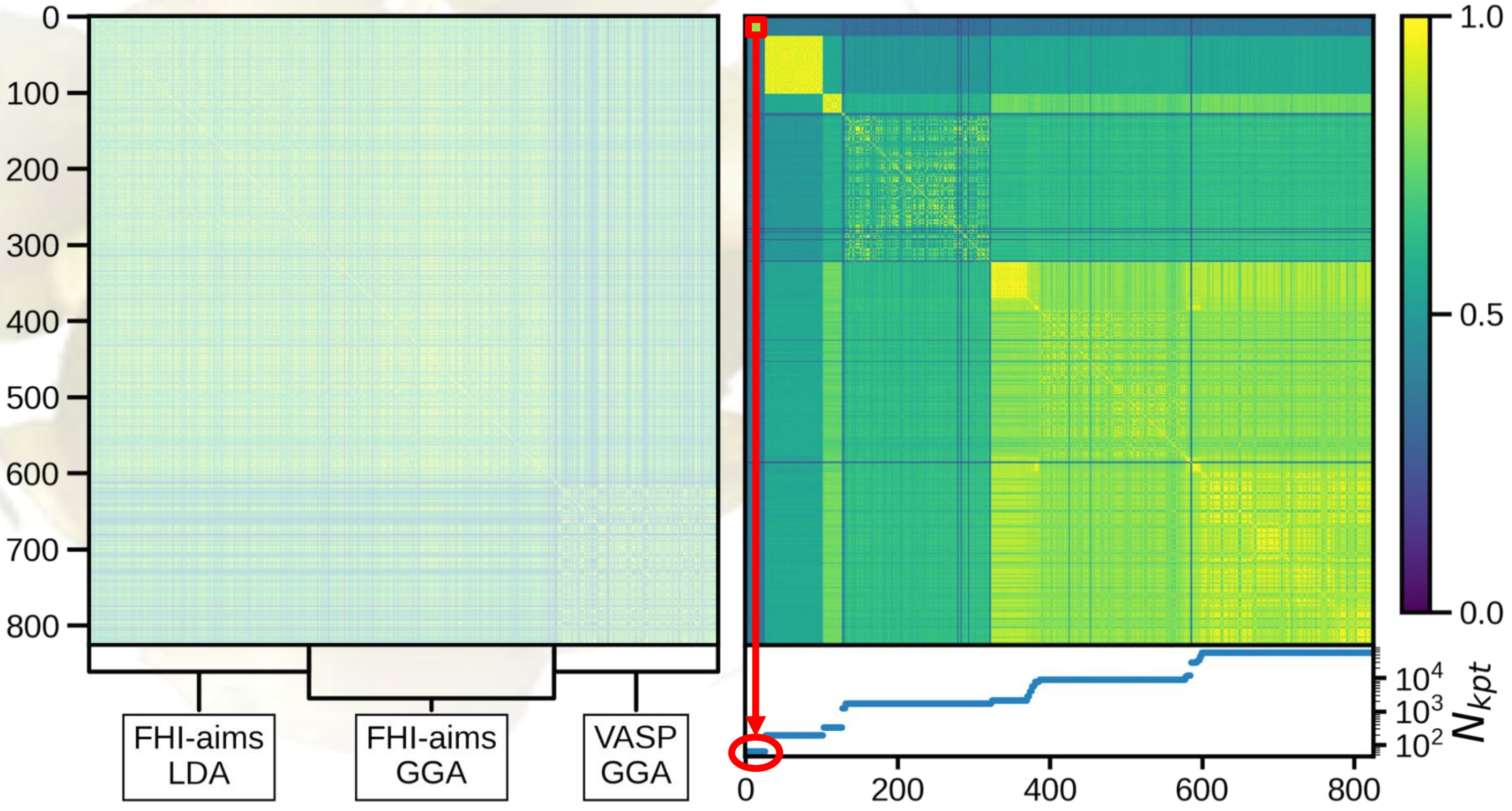

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Code and computational parameters

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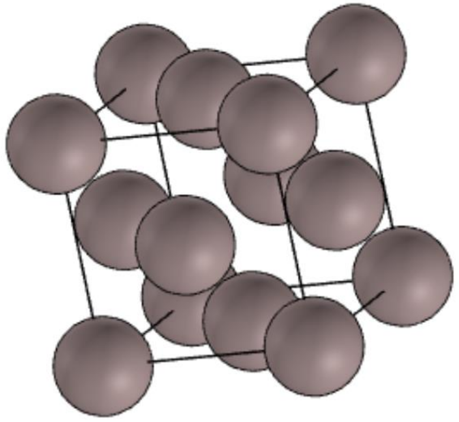

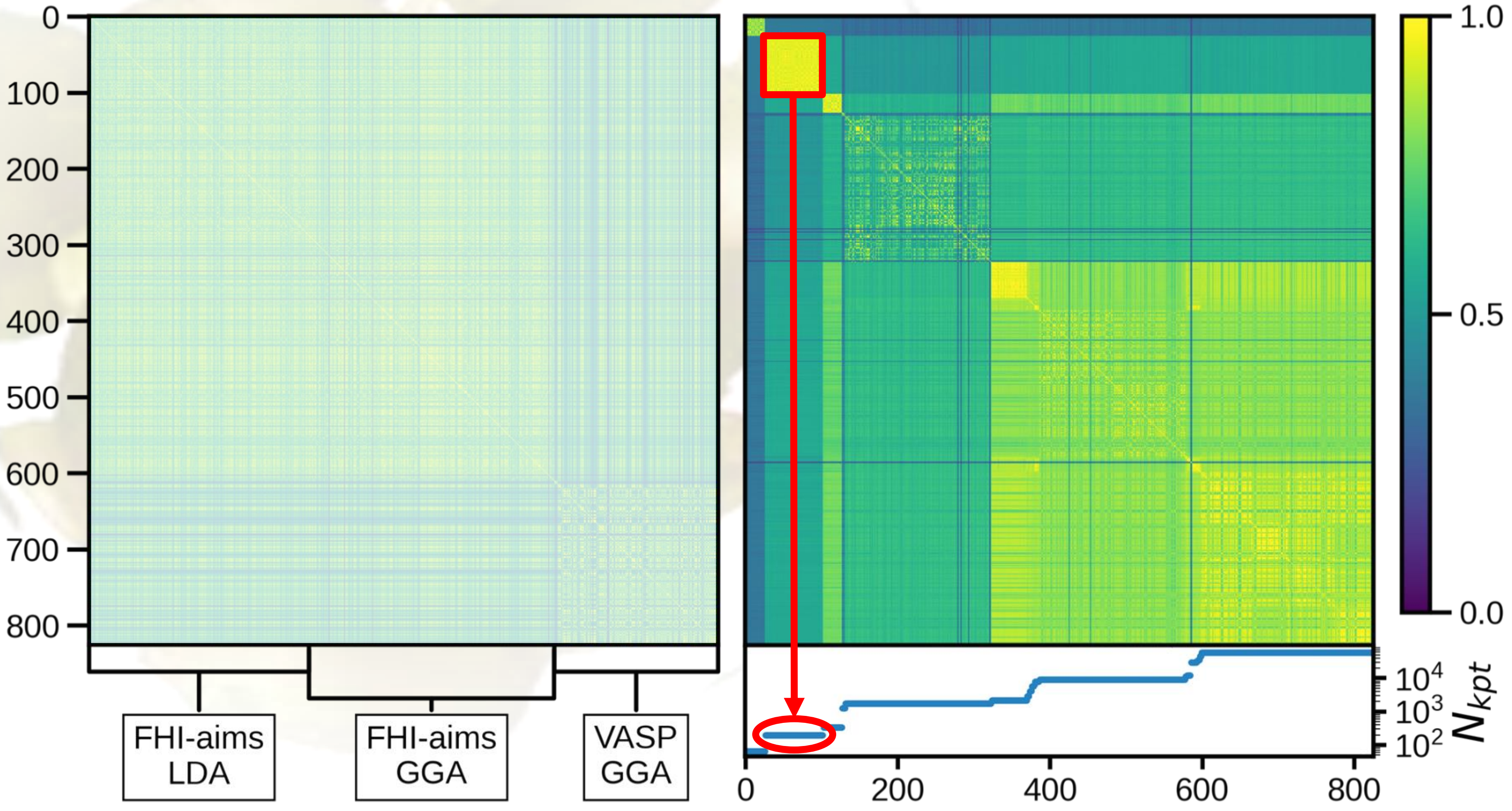

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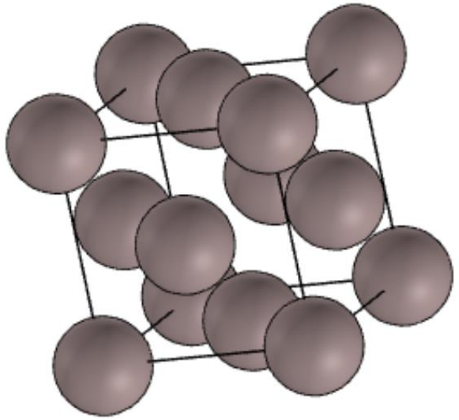

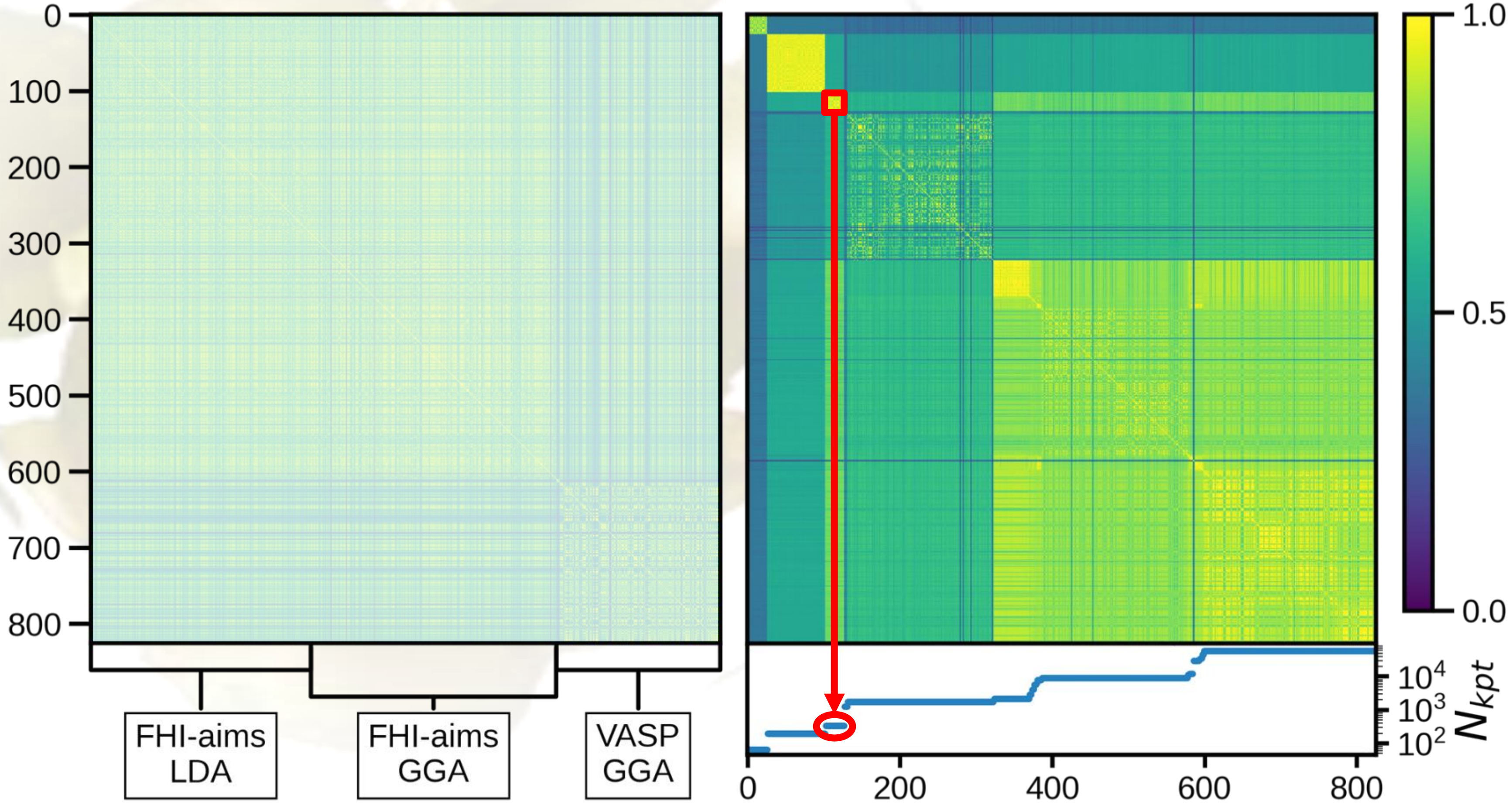

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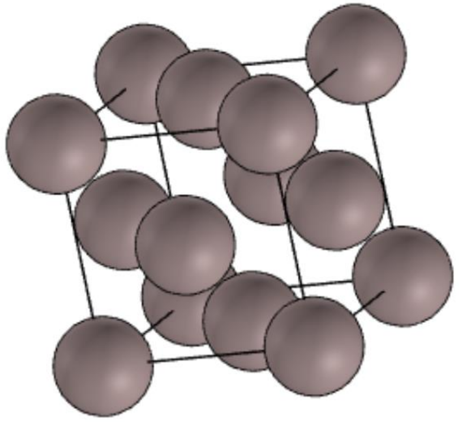

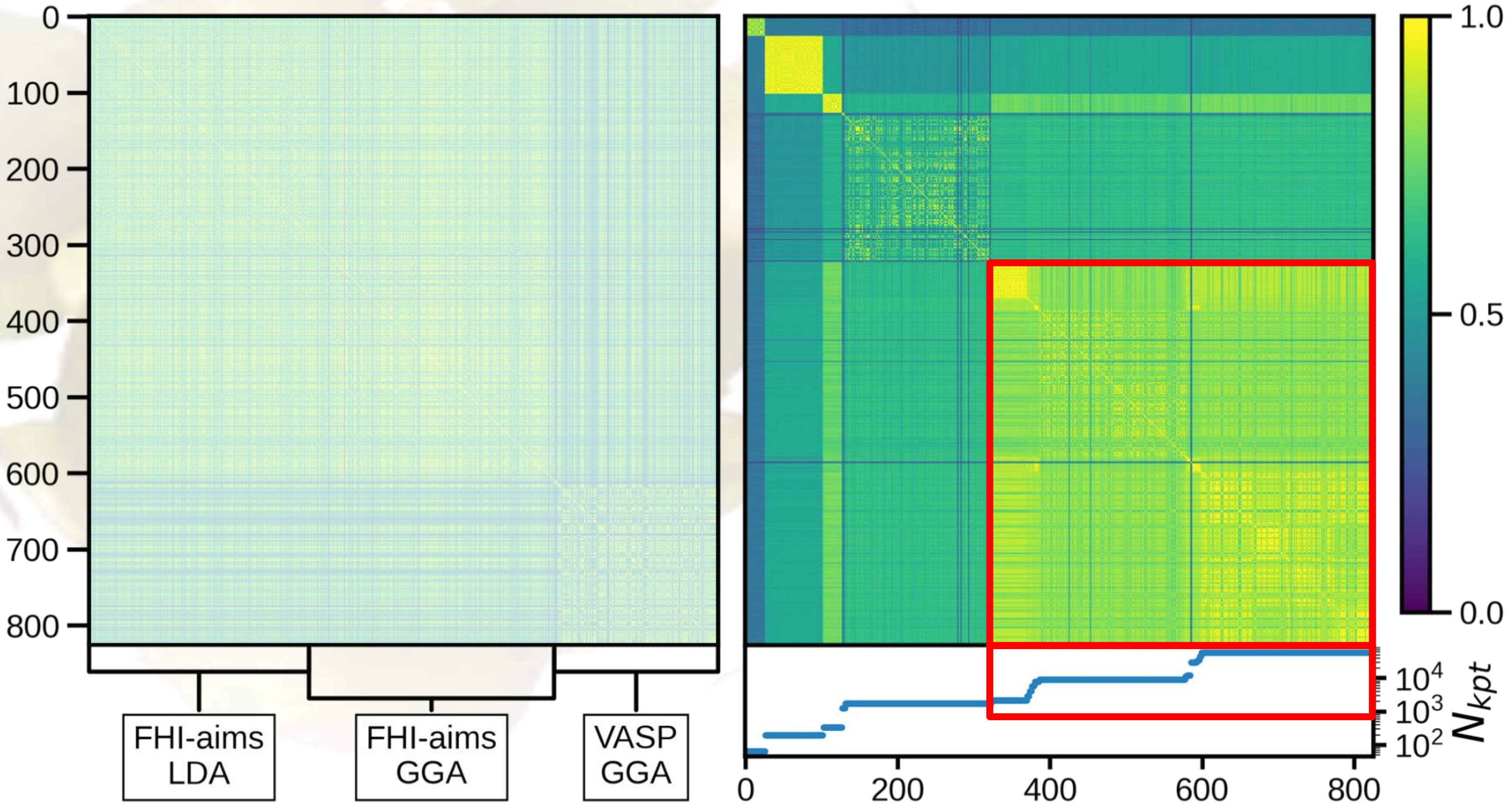

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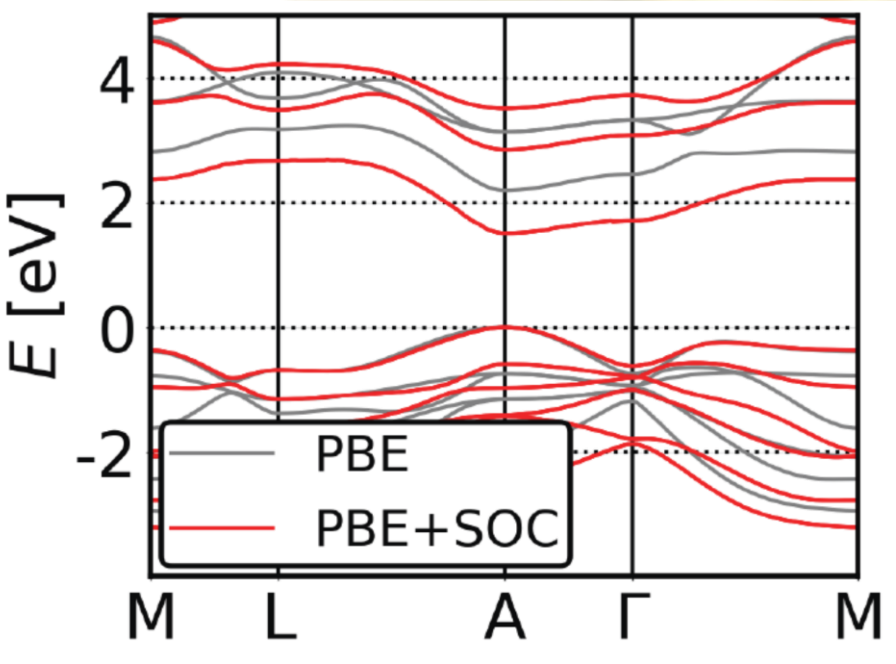
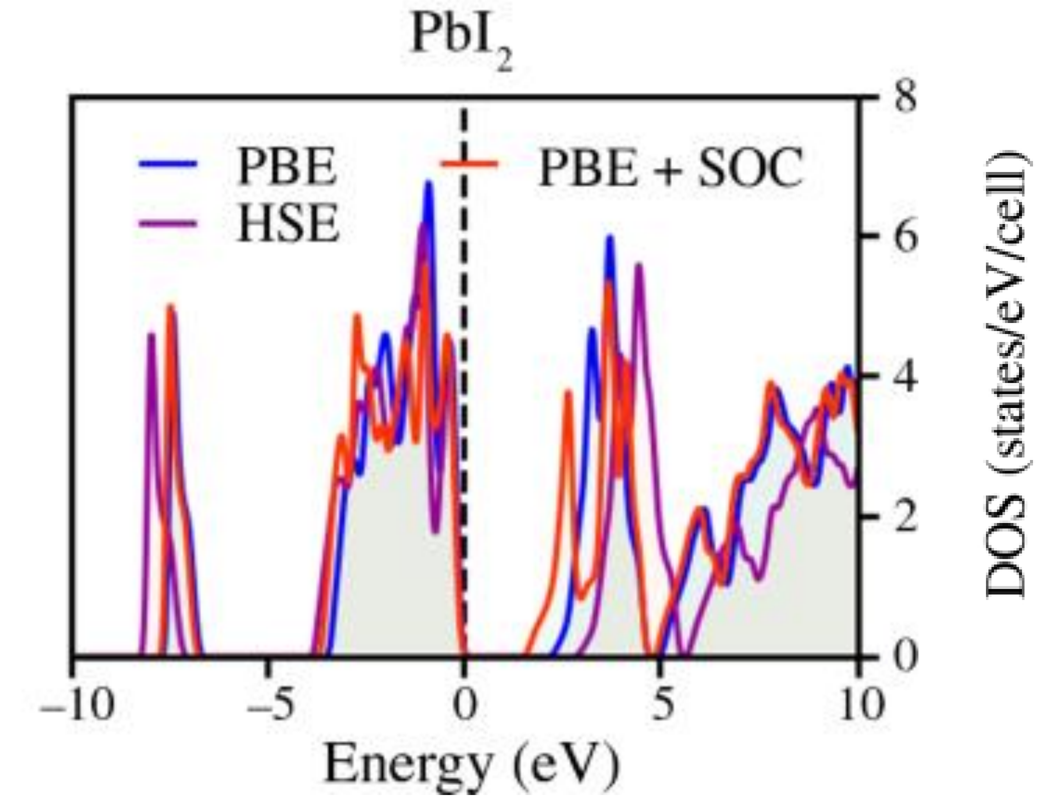
Methodology





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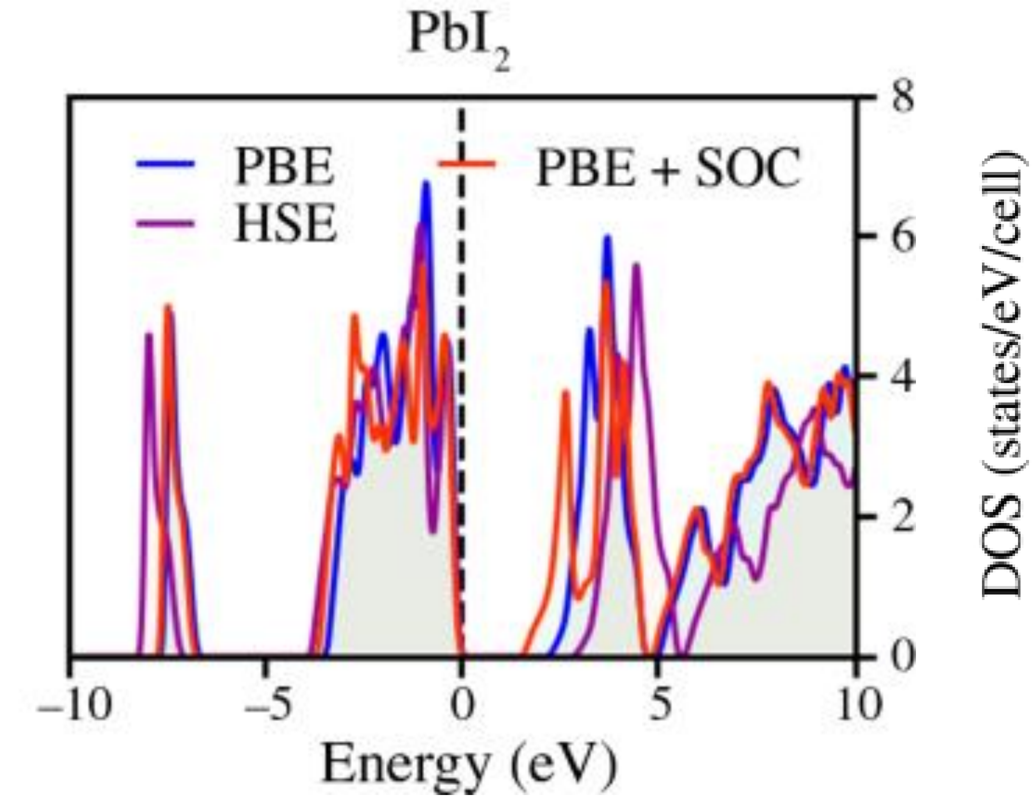
Methodology

PBE vs.	S_{total}	$S_{valence}$	$S_{conduction}$
PBE + SOC	0.71	0.75	0.67
HSE	0.69	0.73	0.45



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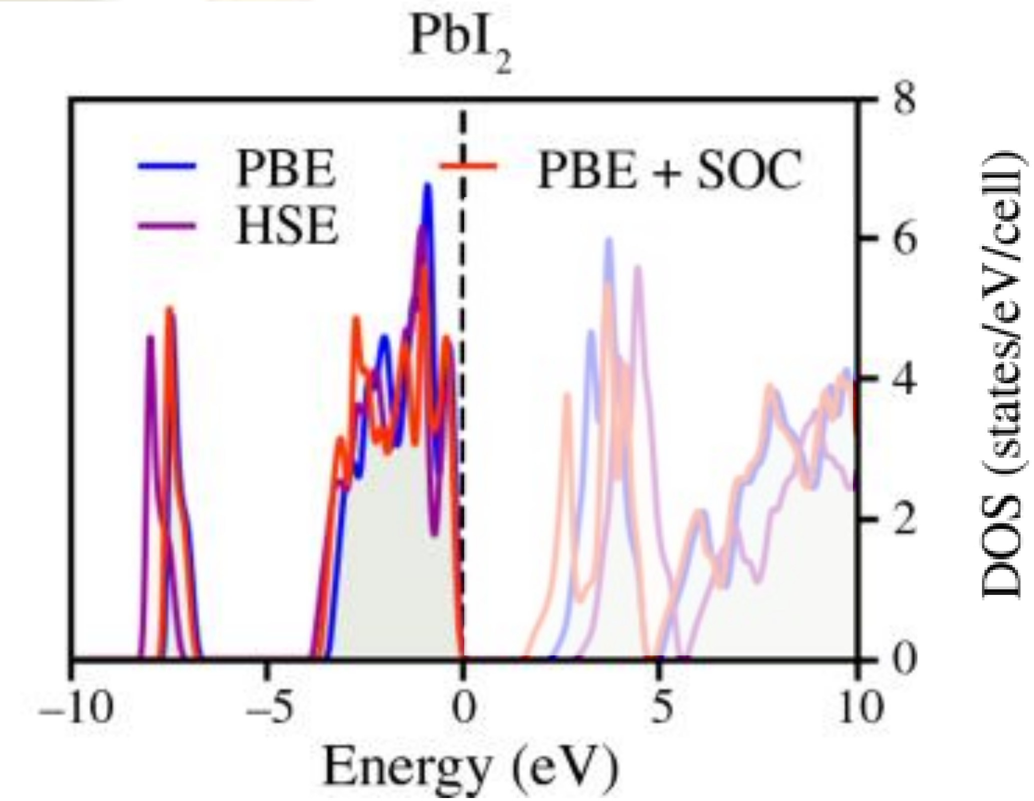

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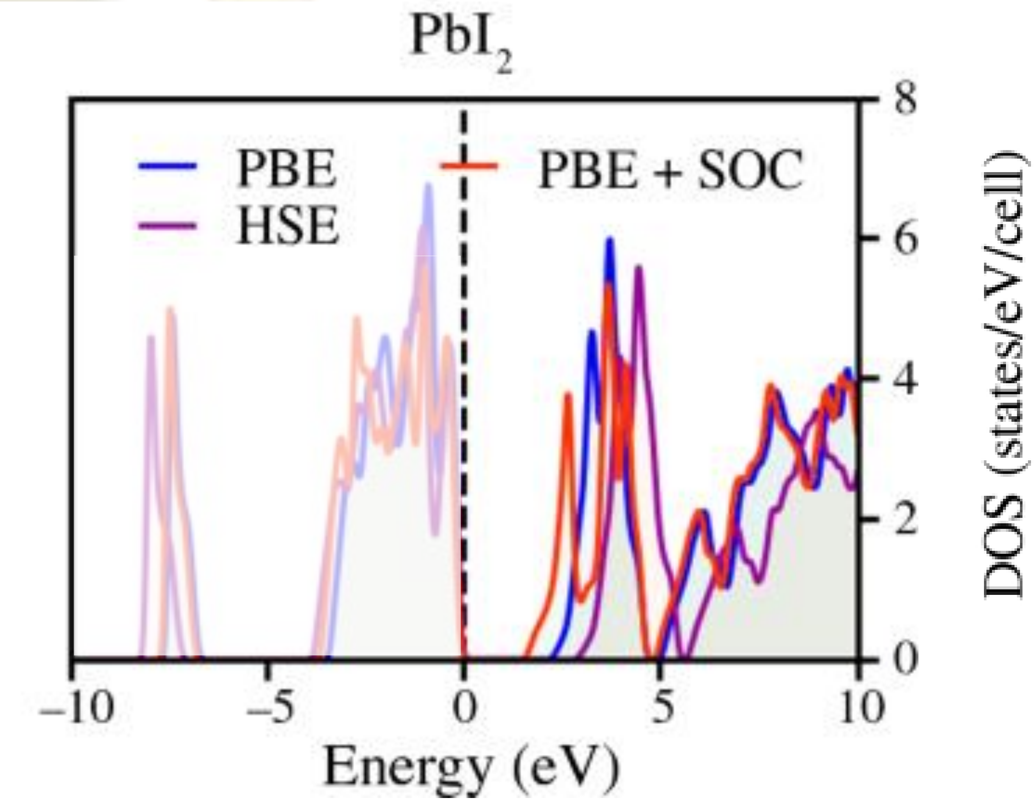

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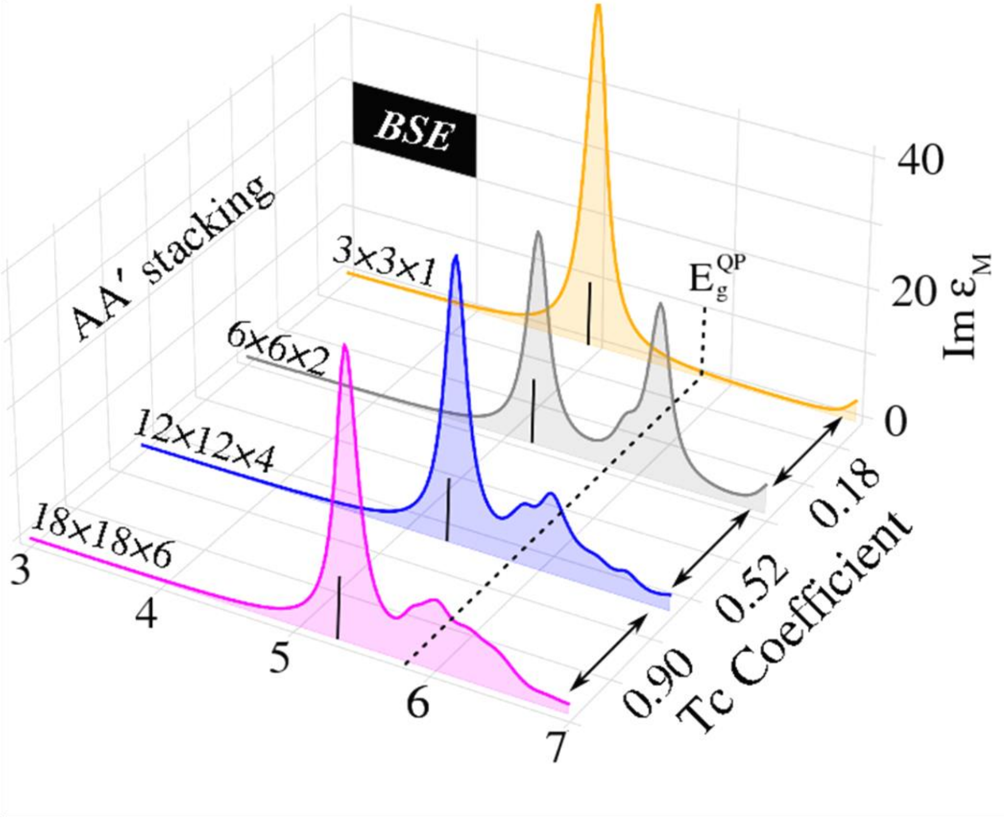
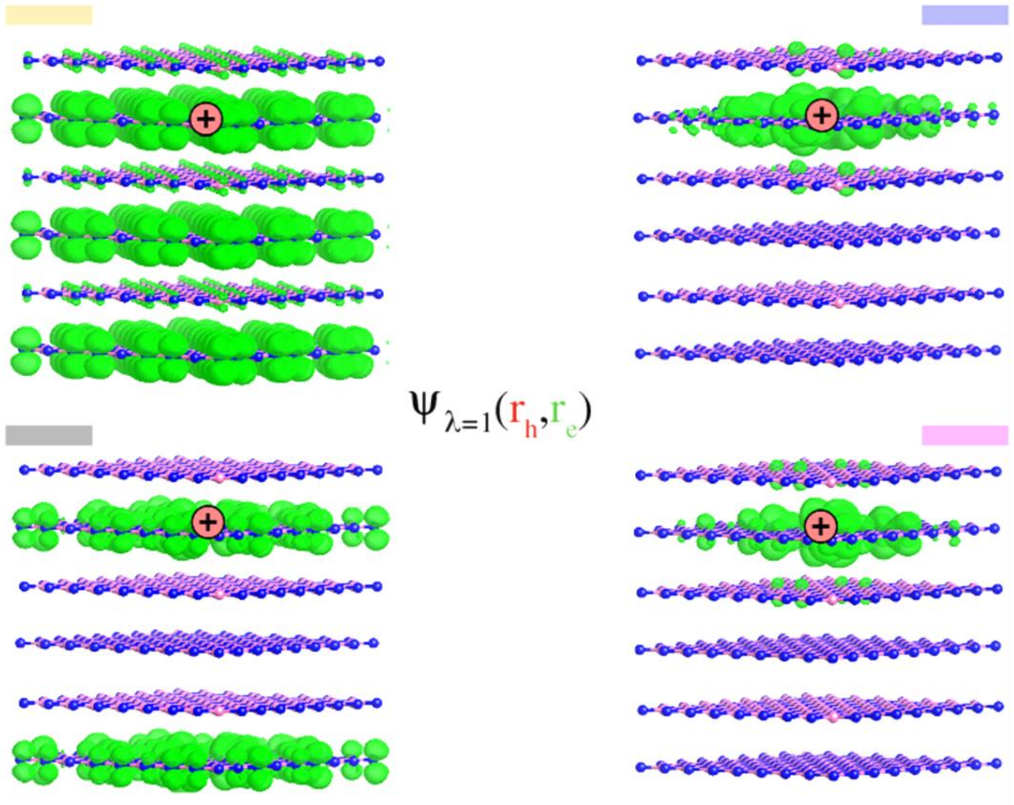
Excitonic spectra

$$\phi^{\lambda}(\mathbf{r}_e,\mathbf{r}_h)=\sum A^{\lambda}_{v c \mathbf{k}}\,\psi^{*}_{v\mathbf{k}}(\mathbf{r}_h)\,\psi_{c\mathbf{k}}(\mathbf{r}_e)$$





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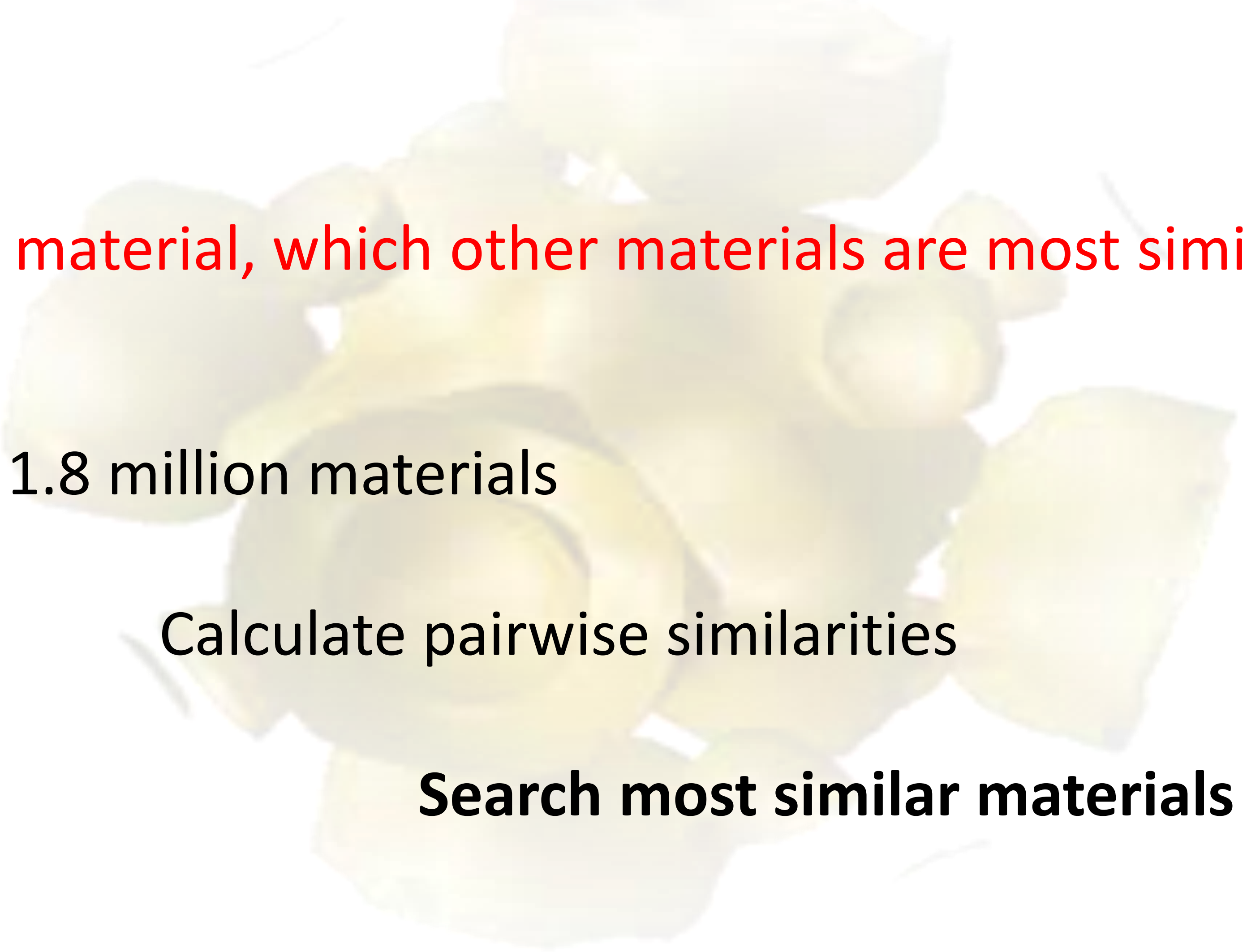
Exploring data spaces

Finding similar materials



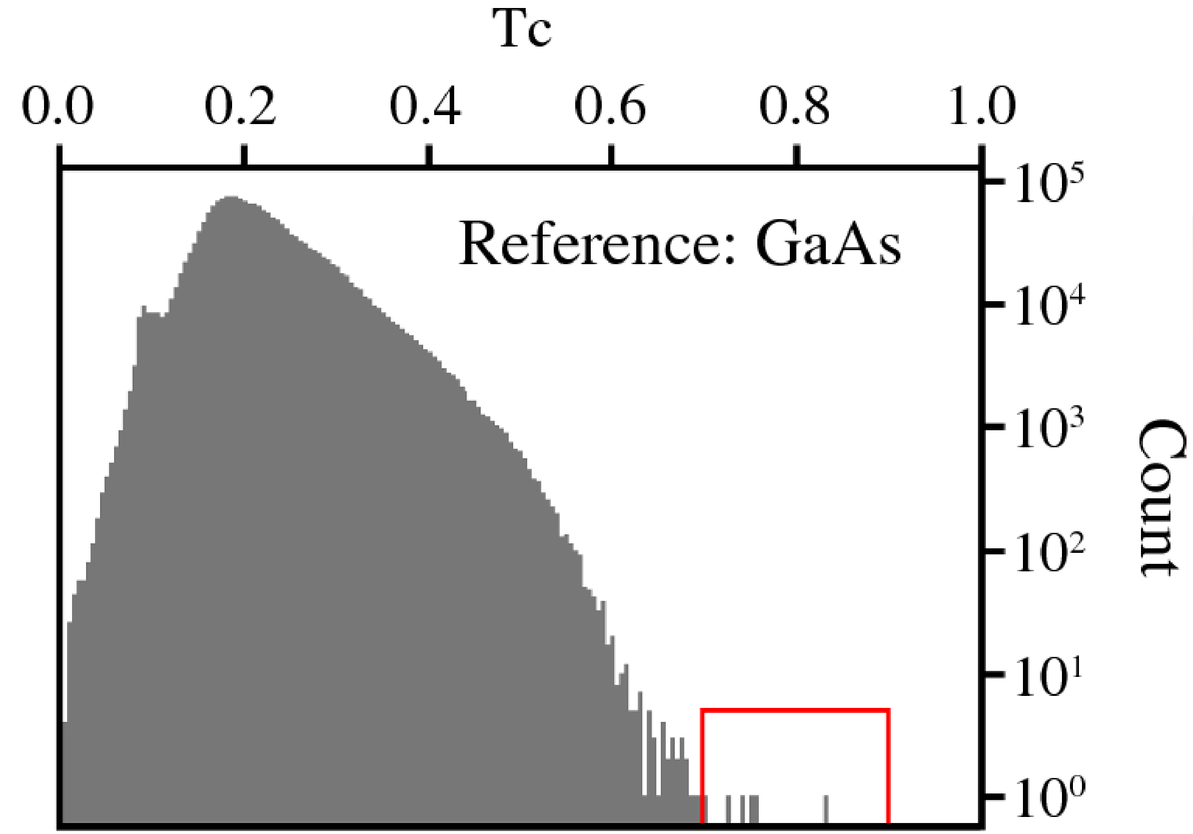
For any material, which other materials are most similar to them?

1.8 million materials

Calculate pairwise similarities

Search most similar materials

Finding similar materials



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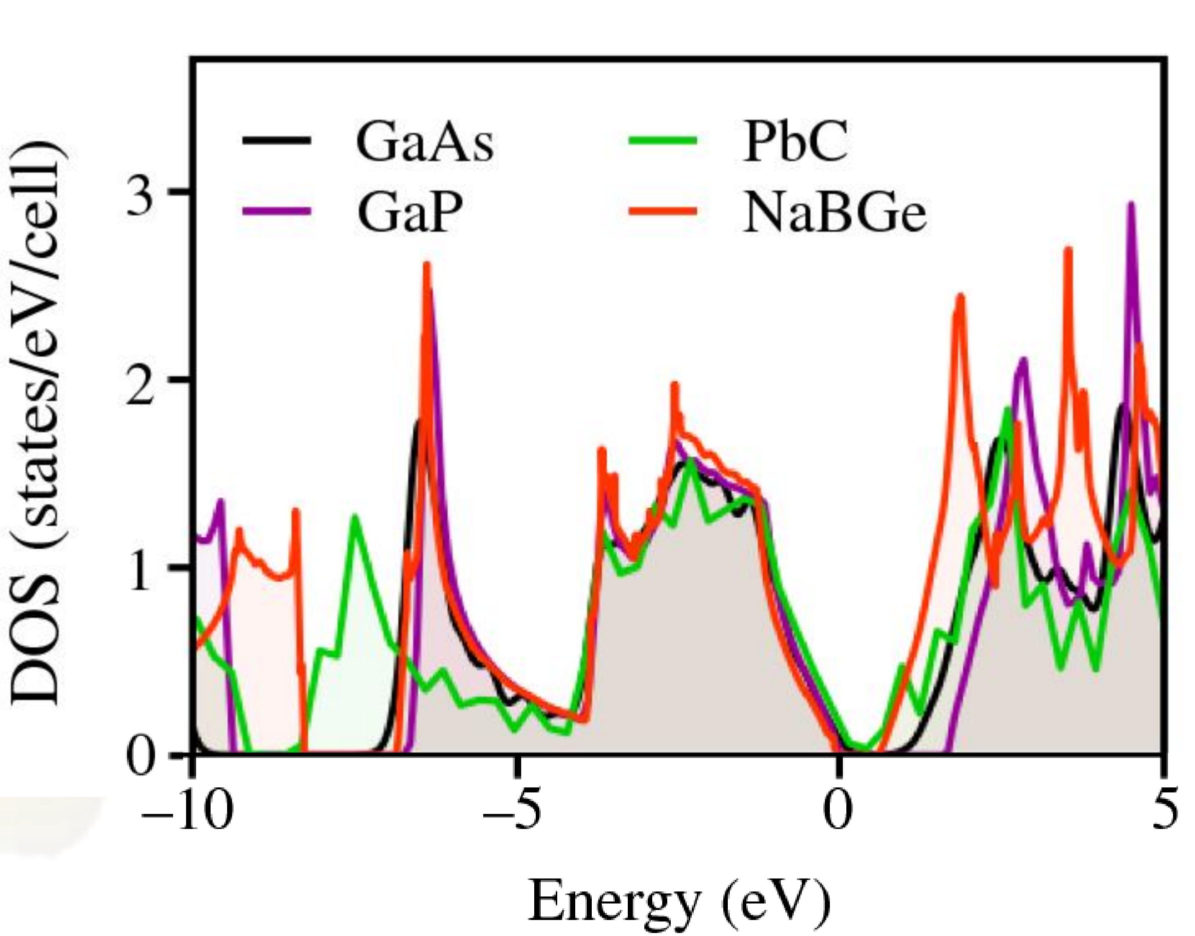
Finding similar materials

Similarity of GaAs to:

GaP:	0.83
PbC:	0.75
NaBGe:	0.74



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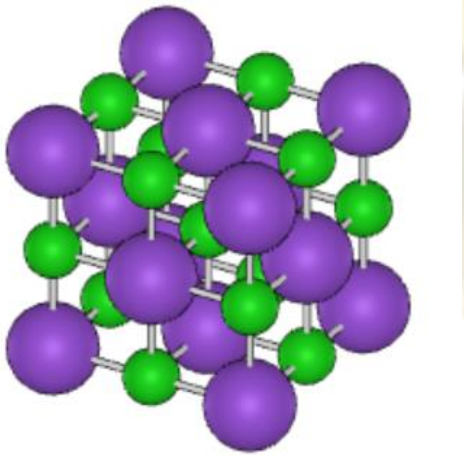
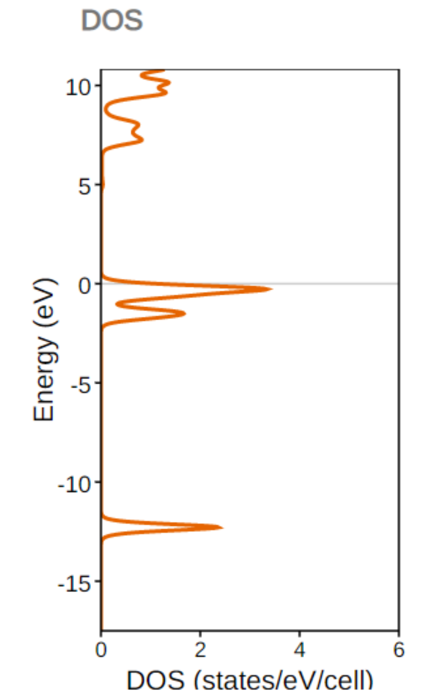
Finding similar materials

NaCl - space group 225

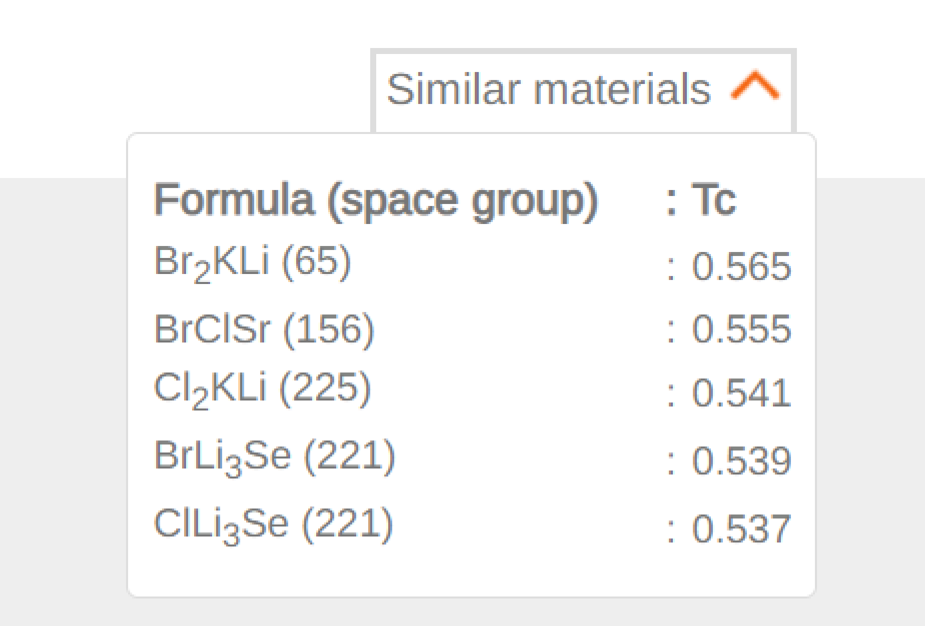




From calculation **zz6kLYmE**

(GGA - VASP)

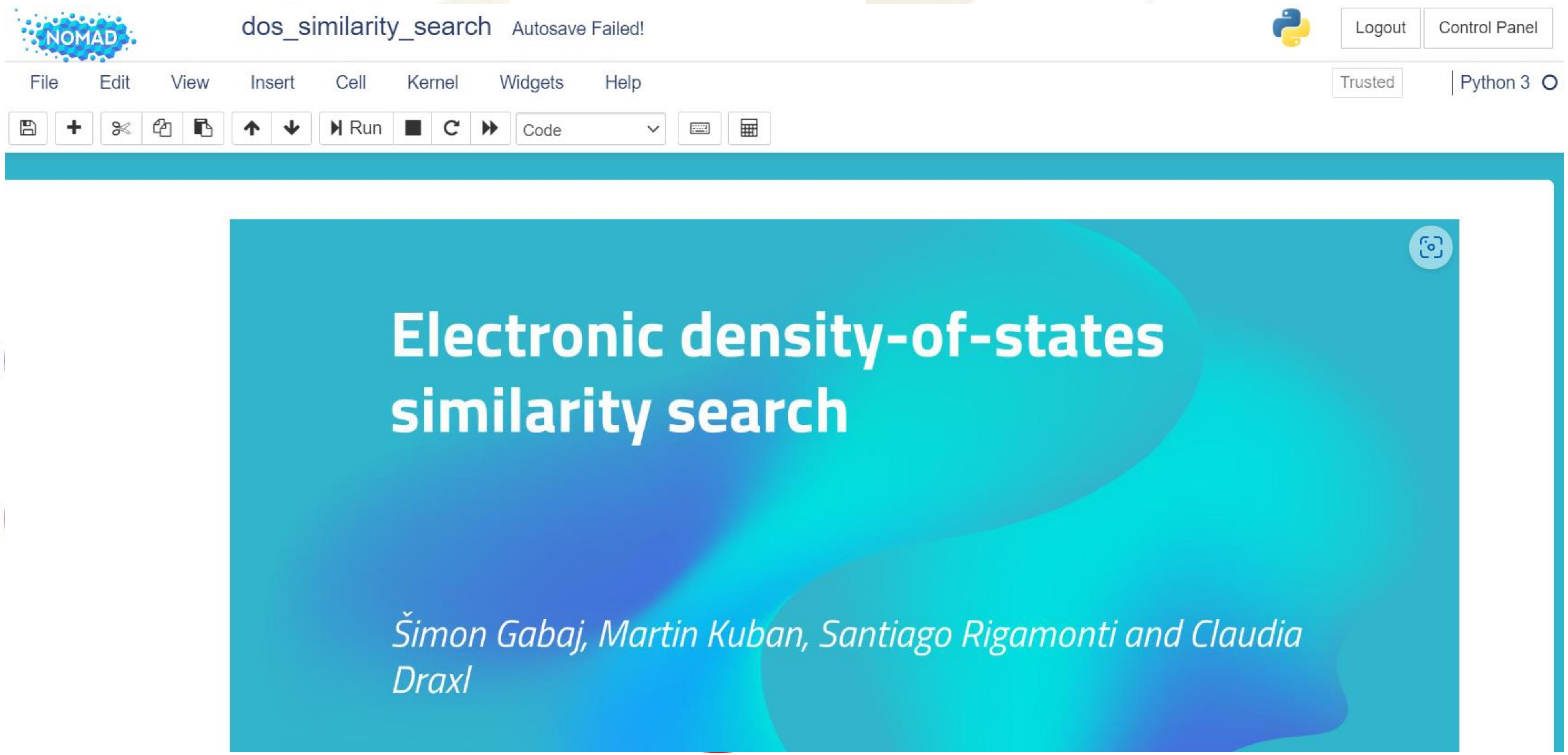
Similar materials



Similar materials

Formula (space group)	: Tc
Br_2KLi (65)	: 0.565
BrClSr (156)	: 0.555
Cl_2KLi (225)	: 0.541
$BrLi_3Se$ (221)	: 0.539
$ClLi_3Se$ (221)	: 0.537

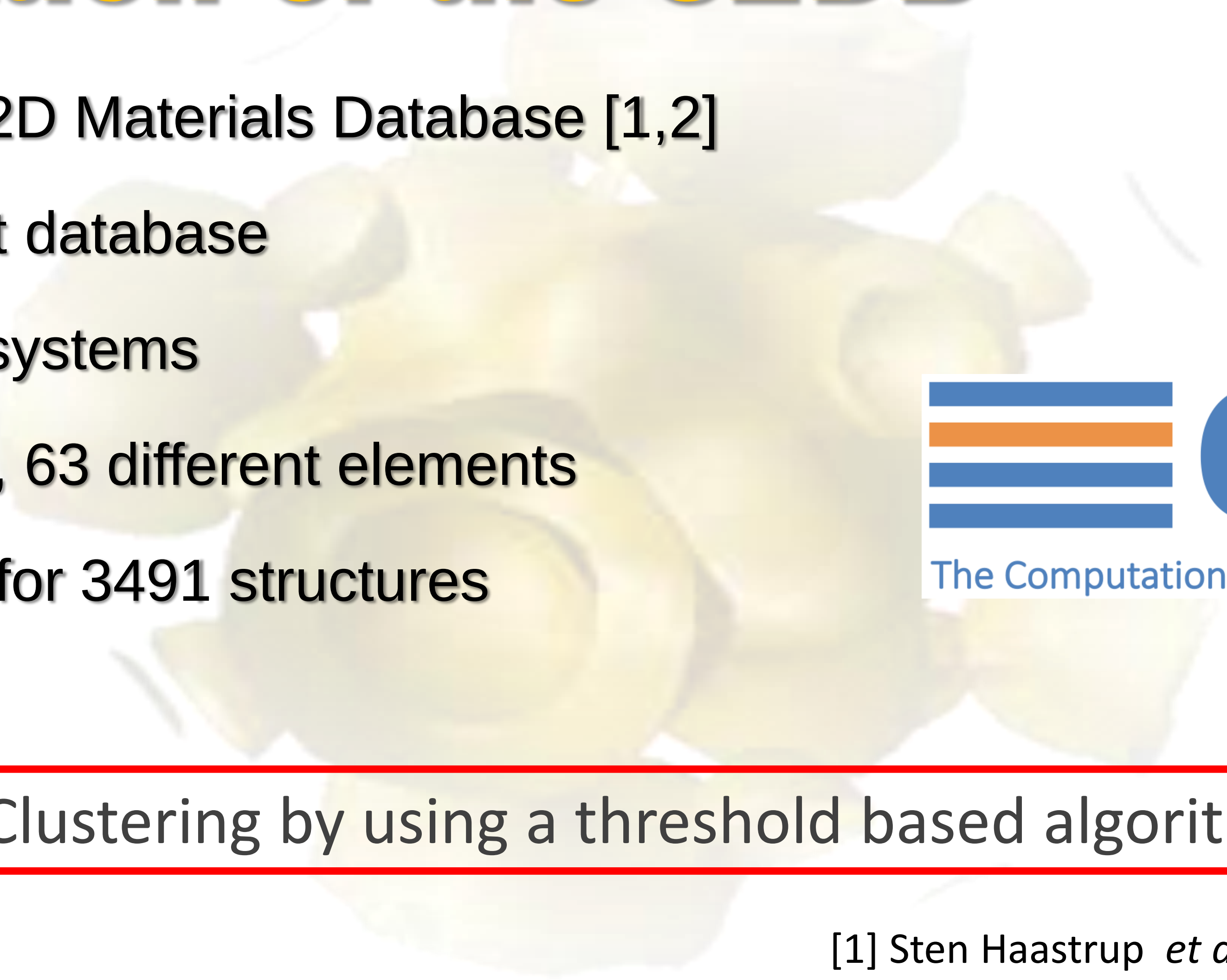
Finding similar materials



Electronic density-of-states similarity search

Šimon Gabaj, Martin Kuban, Santiago Rigamonti and Claudia Draxl

Exploration of the C2DB



Computational 2D Materials Database [1,2]

High-throughput database

Atomically thin systems

4047 structures, 63 different elements

Projected DOS for 3491 structures

C2DB

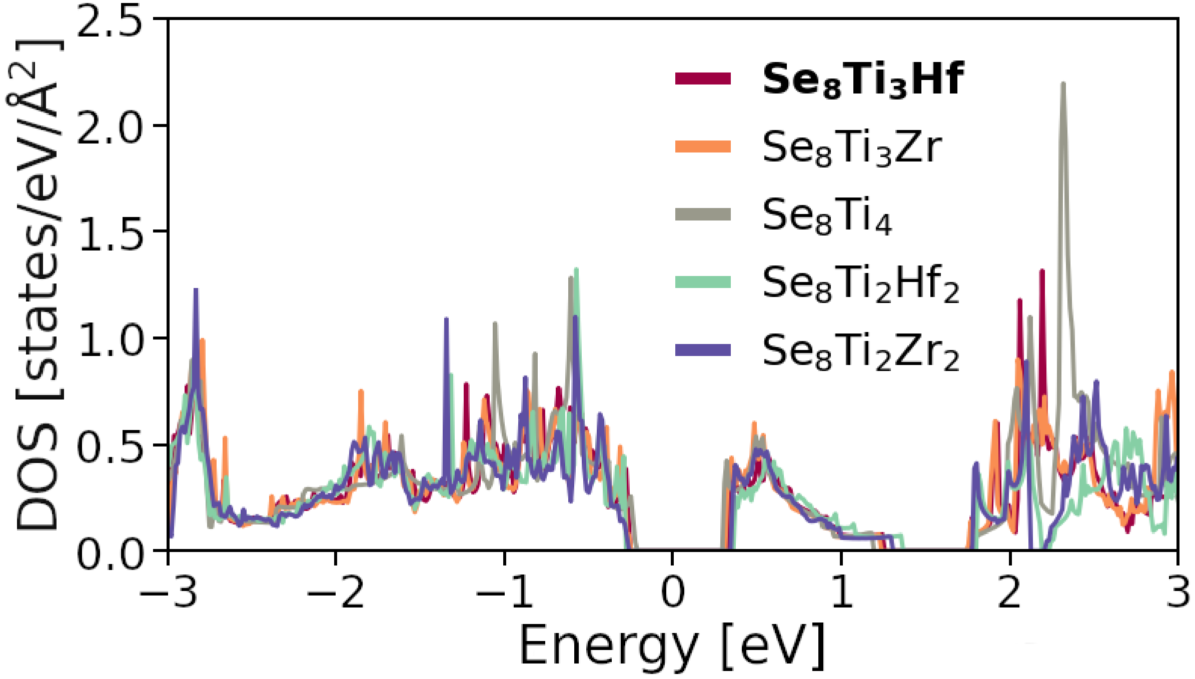
The Computational 2D Materials Database

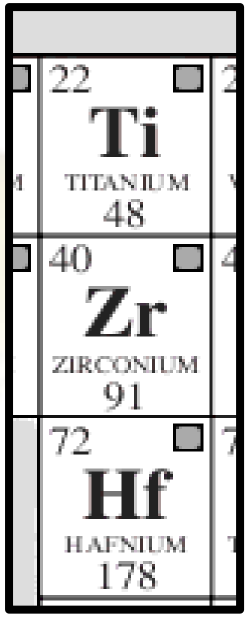
Clustering by using a threshold based algorithm

[1] Sten Haastrup *et al.*, 2D Materials 5, 042002 (2018)

[2] M. N. Gjerding *et al.*, 2D Materials 8, 044002 (2021)

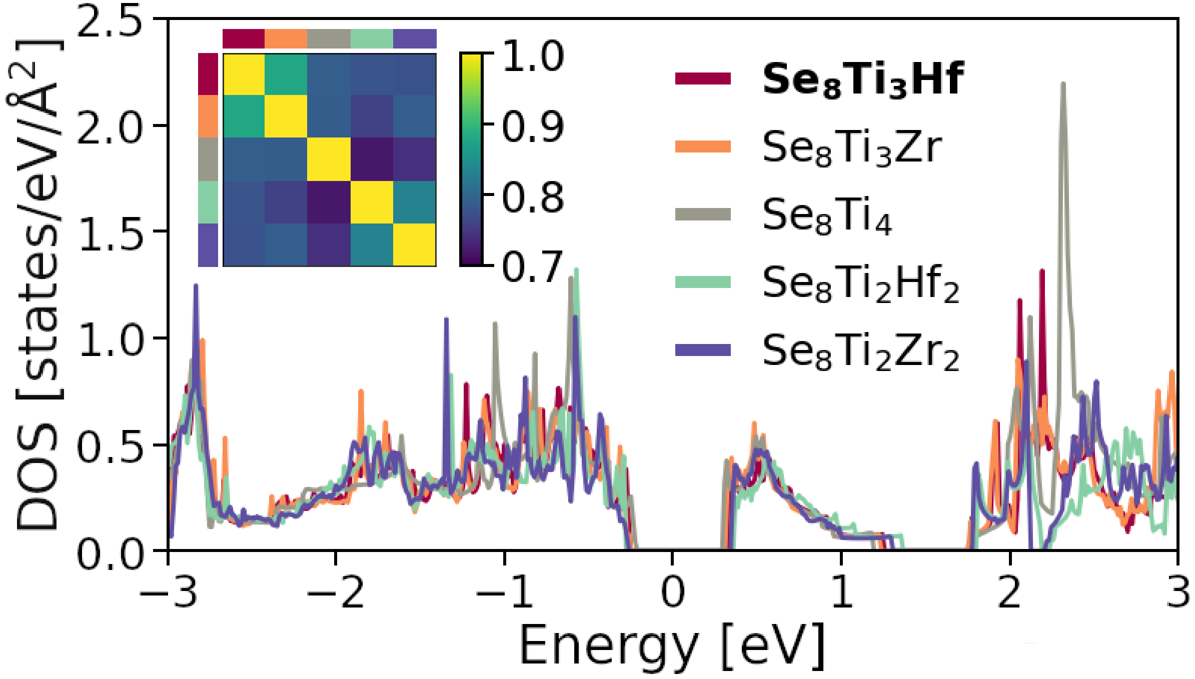
Cluster analysis

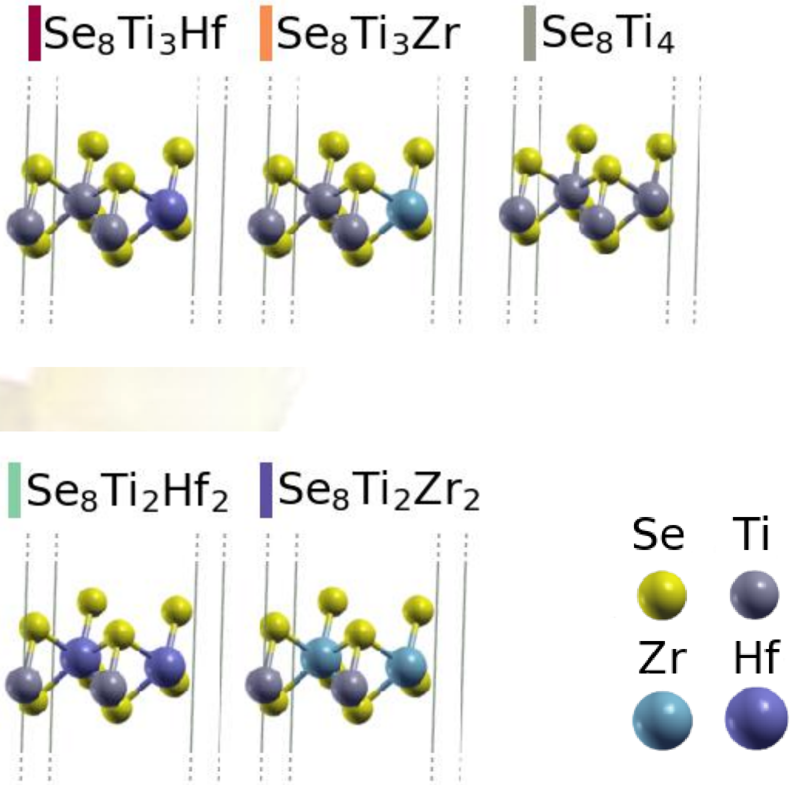




M. Kuban *et al.* Sci Data **9**, 646 (2022).

Cluster analysis





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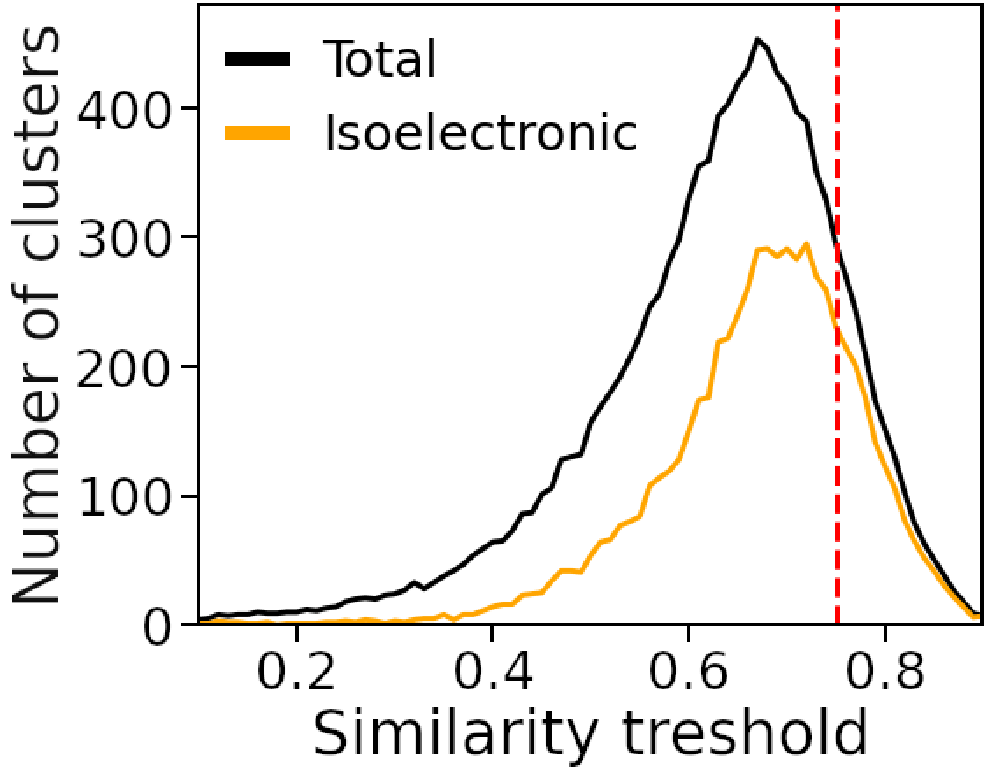
Isoelectronic clusters

Descriptor for isoelectronic clusters:

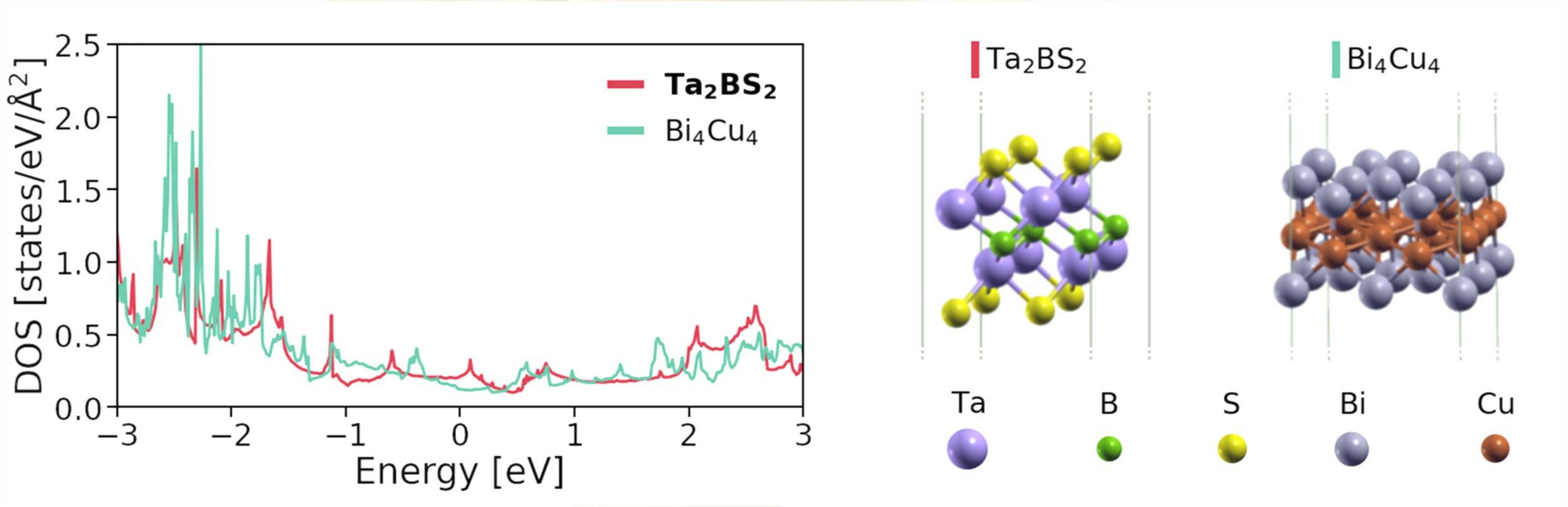
$$\bar{c}_m = \frac{1}{N_{Atoms}} \sum_{i=1}^{N_{Atoms}} c_i$$

230 isoelectronic clusters (78%)



M. Kuban *et al.* Sci Data **9**, 646 (2022).

Outliers



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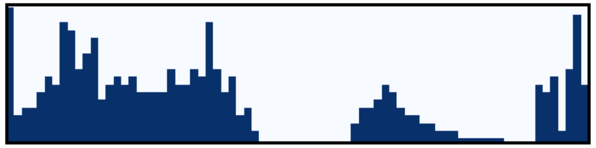
Conclusions

Spectral fingerprint to quantitatively evaluate the similarity of spectra

Quality assessment:

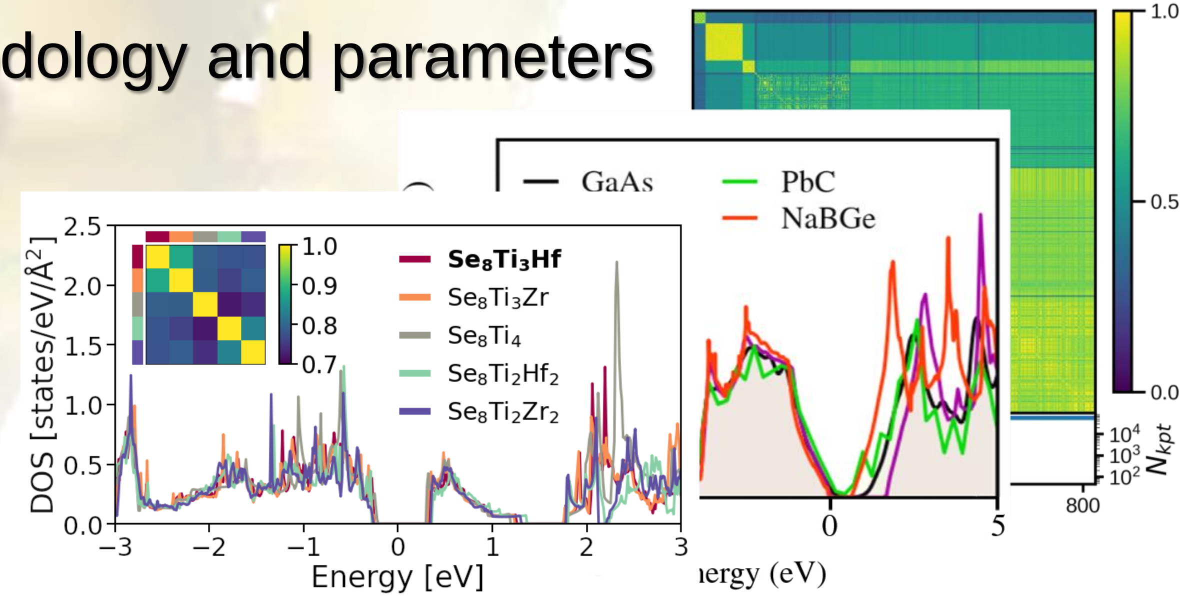
Measuring the impact of methodology and parameters



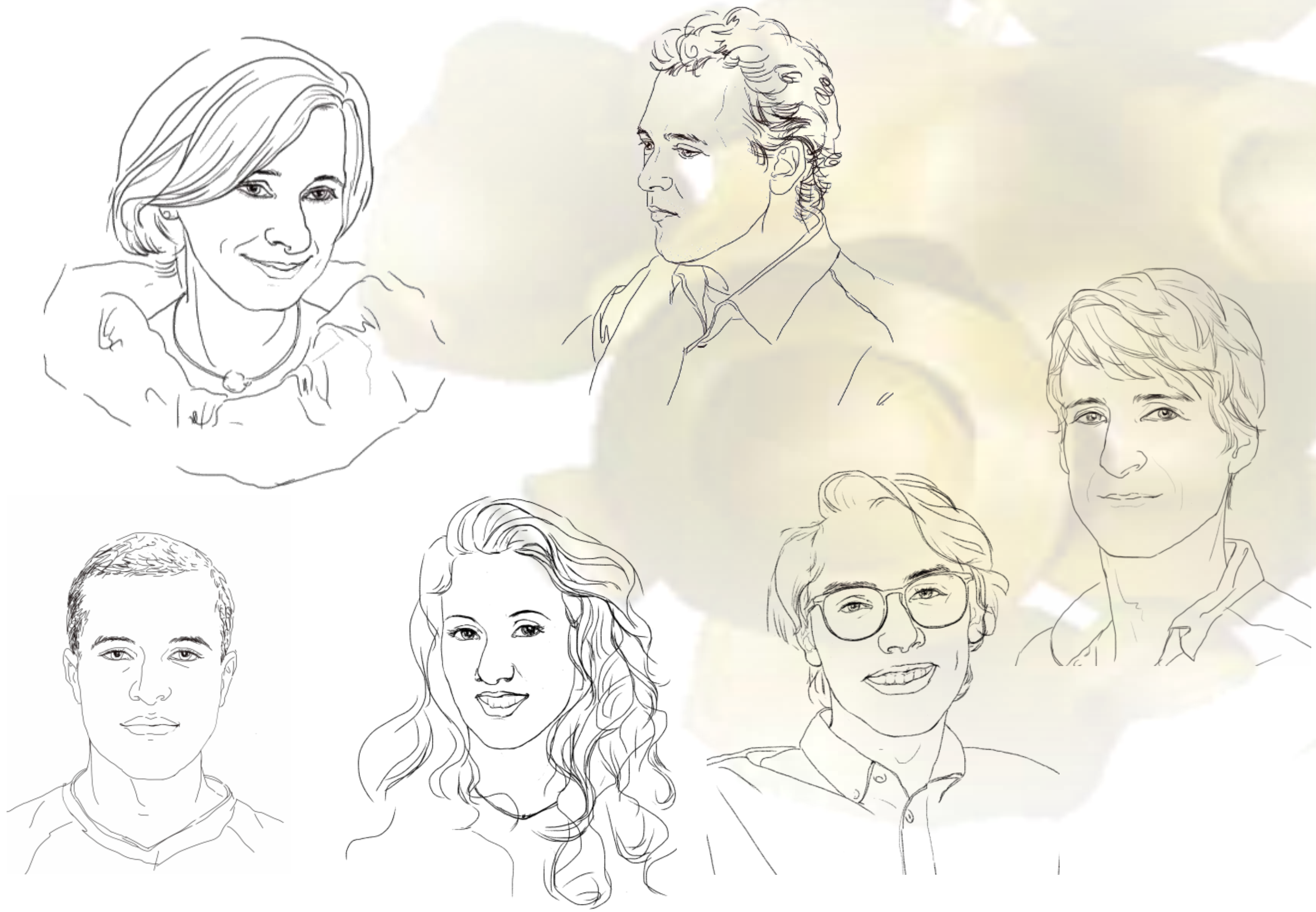
Data analytics:

Finding similar materials

Unsupervised learning



Acknowledgements



FONDA

FAIRmat

NOMAD

NOVEL MATERIALS DISCOVERY

NOMAD

Further reading

Kuban, M., Rigamonti, S., Scheidgen, M., Draxl, C., Density-of-states similarity descriptor for unsupervised learning from materials data. *Sci Data* **9**, 646 (2022)

Kuban, M., Gabaj, Š., Aggoune, W. *et al.* Similarity of materials and data-quality assessment by fingerprinting. *MRS Bulletin* **47**, 991–999 (2022).

NOMAD AI Toolkit Tutorial:

`https://nomad-lab.eu/aitoolkit/tutorial-dos-similarity`