Machine Learning in Chemistry now and in the future

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The same team ran away with the competition in **CASP 14** in 2020, leading CASP co-founder John Moult to conclude "In some sense the problem is solved"

Rise of the (chemical) machines

The team was Alphafold, by 

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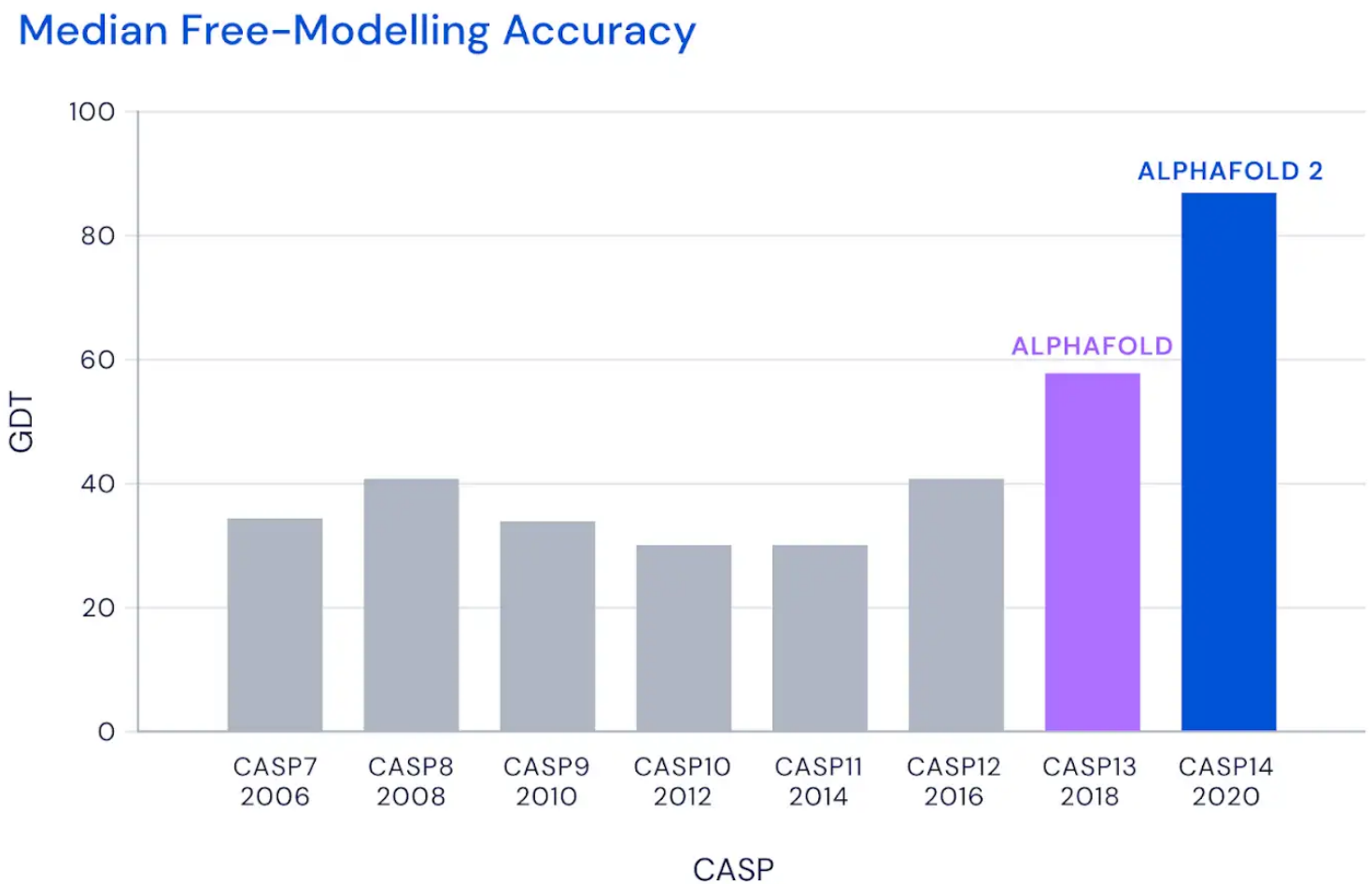
The team was Alphafold, by DeepMind.



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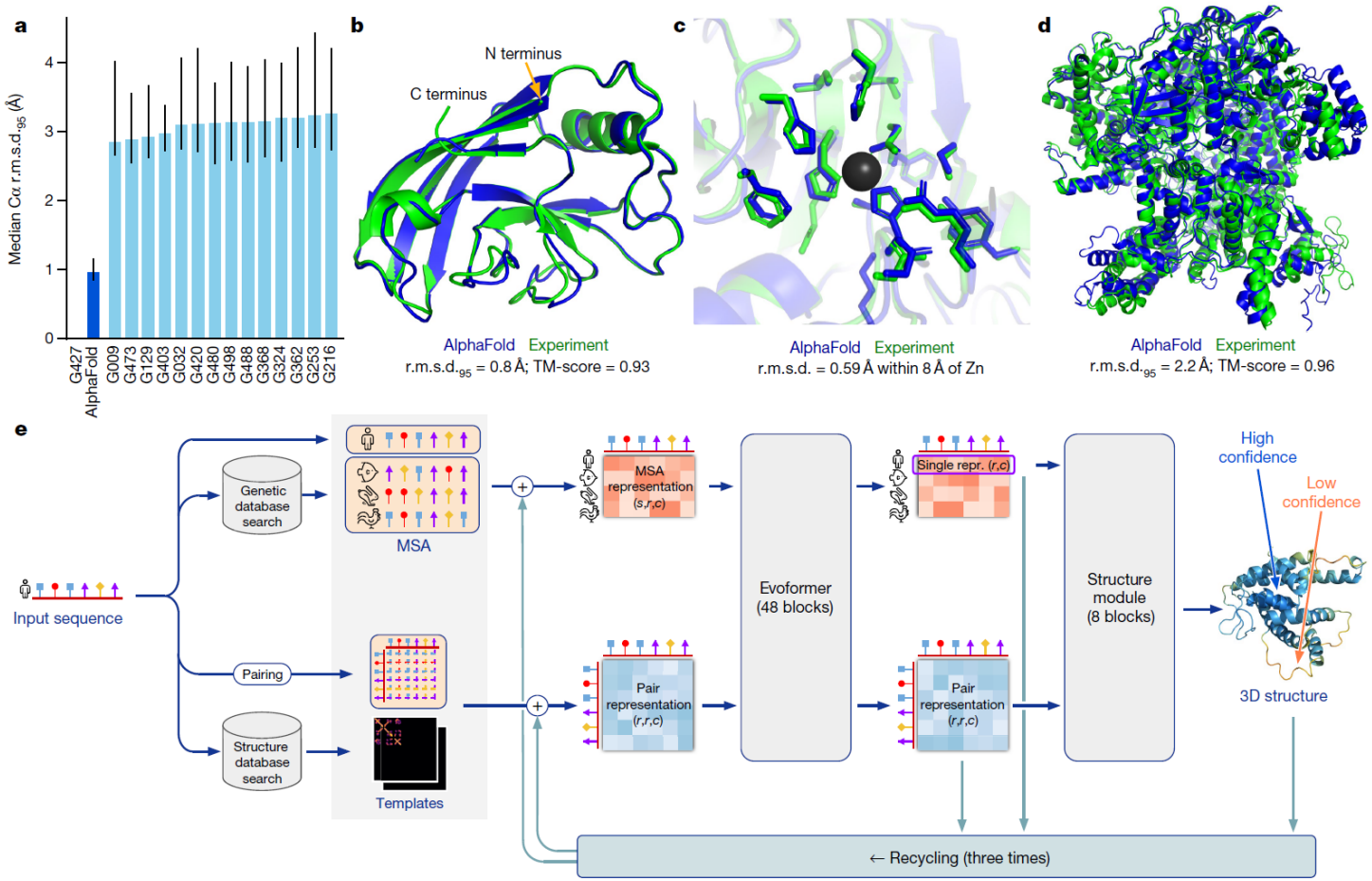

Senior, A.W., *et al.*, *Nature*, 577: 706–710, 2020. Jumper, J., *et al.*, *Nature*, 596: 583–589, 2021.

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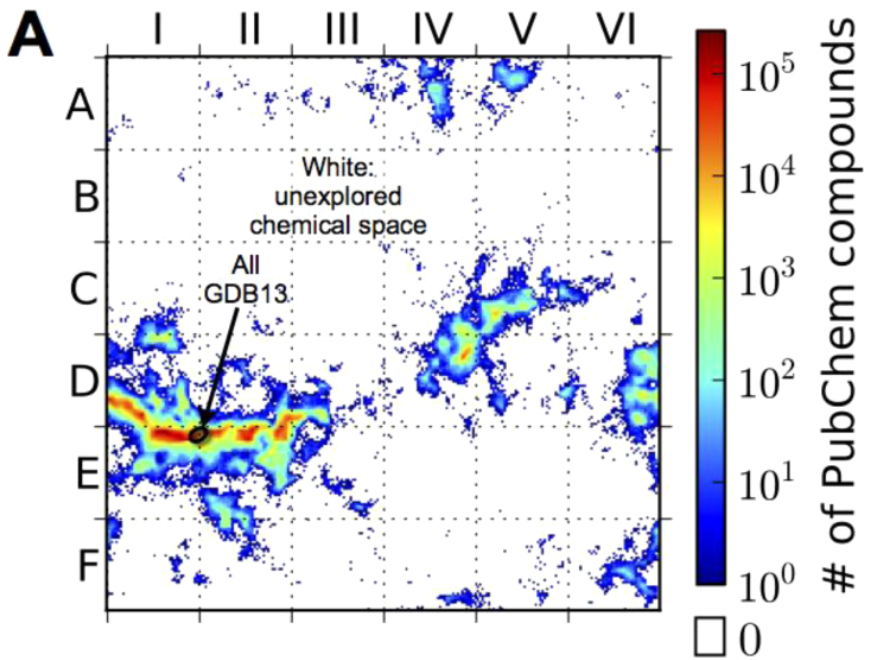
This is probably a bit strong, but all scientists generate data as a product. ML provides new, powerful ways to exploit this information.

Motivation: chemical discovery

Why is ML transforming chemisty?

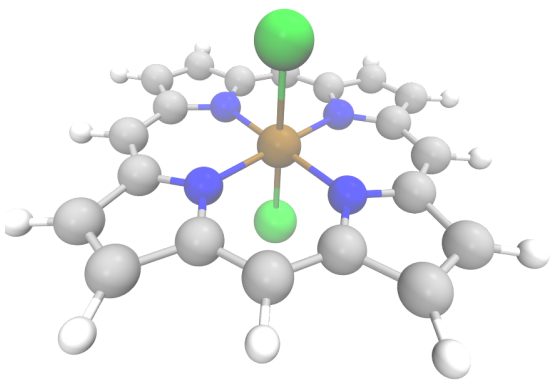
The space of possible chemistries is incredibly vast, with $\mathcal{O}(10^{60})$ small organic molecules.

All potentially undiscovered medicines, catalysts and materials are somewhere, out in this huge space.



Virshup *et al.*, *J. Am. Chem. Soc.*, 135(19): 7296–7303, 2013.

Why ML in chemical sciences?



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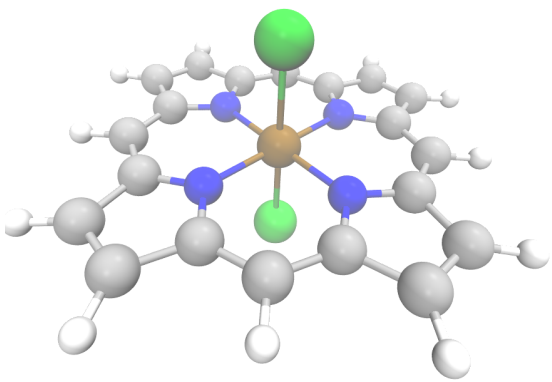

property

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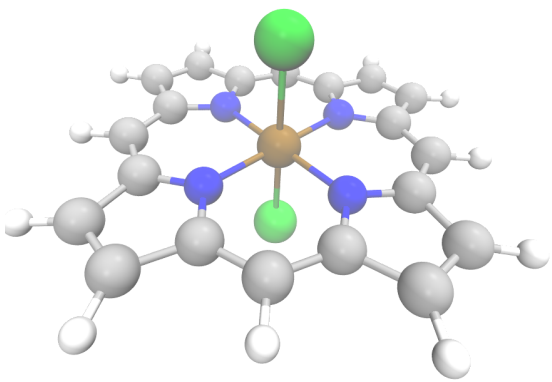

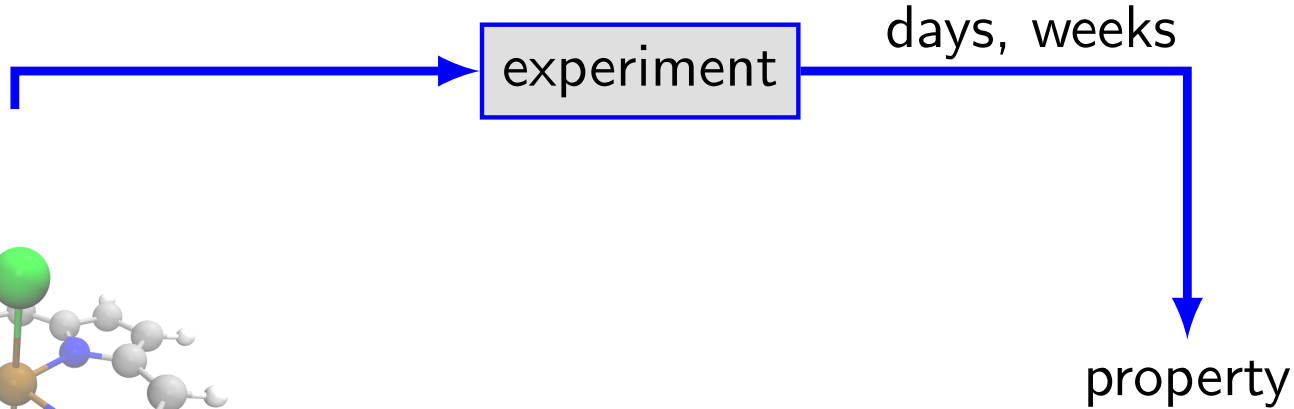

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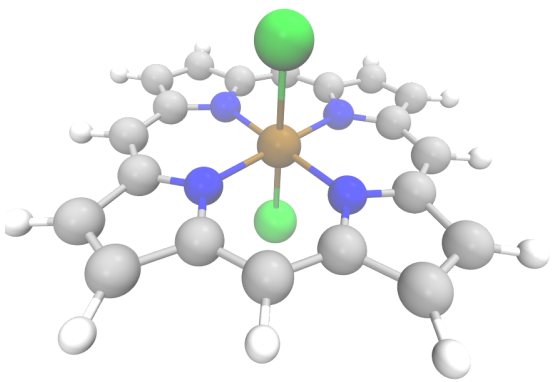

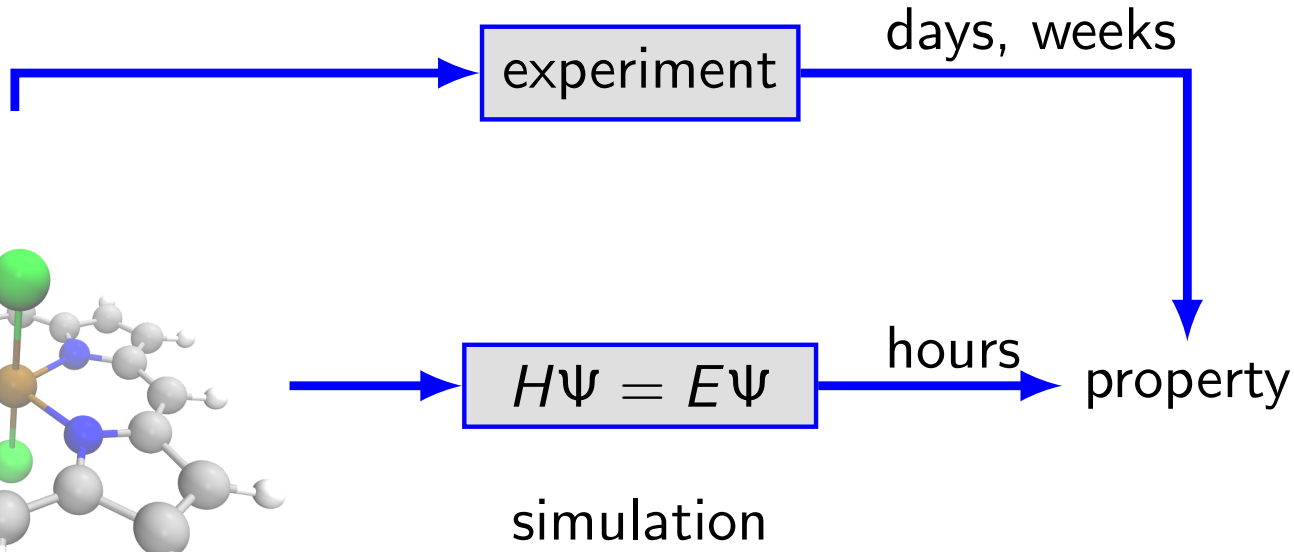

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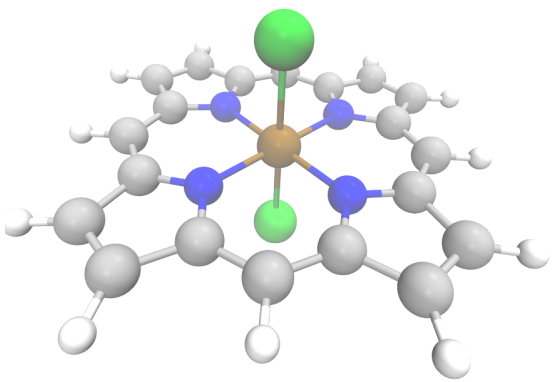

Why does ML work well in chemical sciences?

machine learning methods

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computer vision

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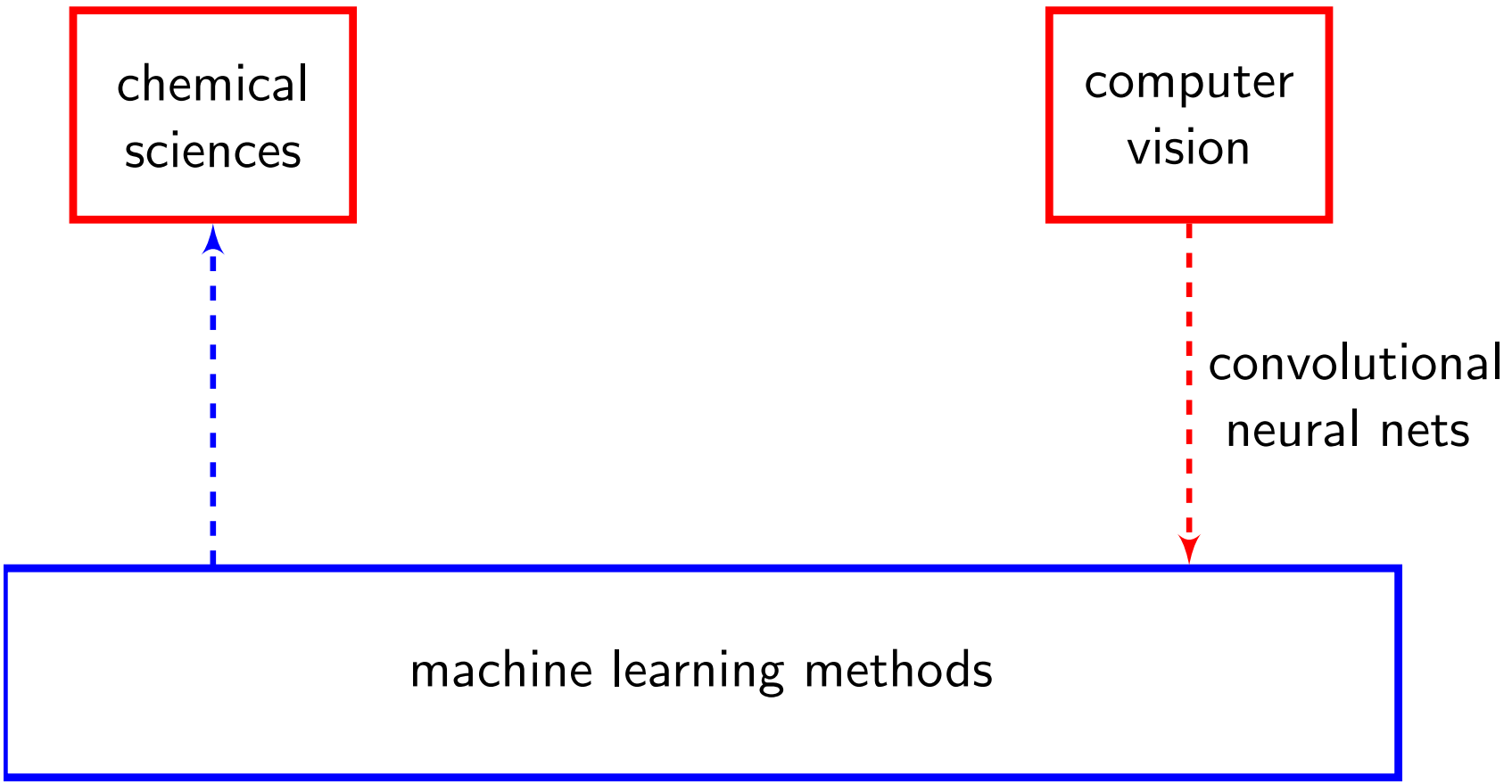

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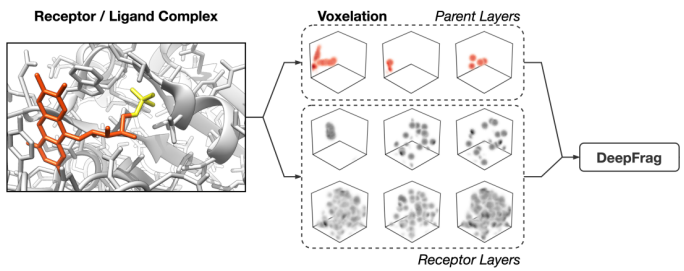

convolutional neural nets

Green, H., *et al.*, bioRxiv 2021.01.07.425790, 2021.

machine learning methods

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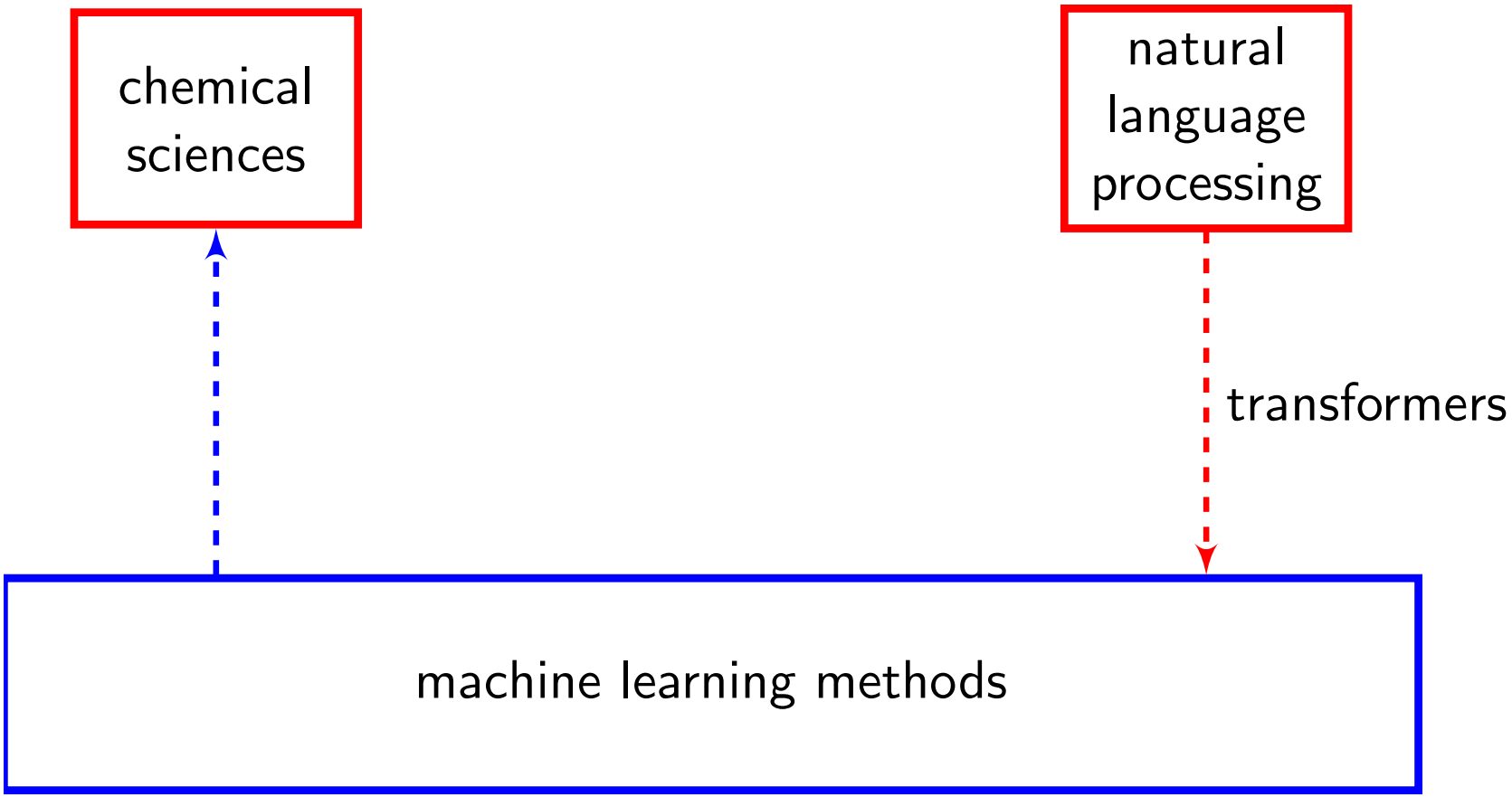

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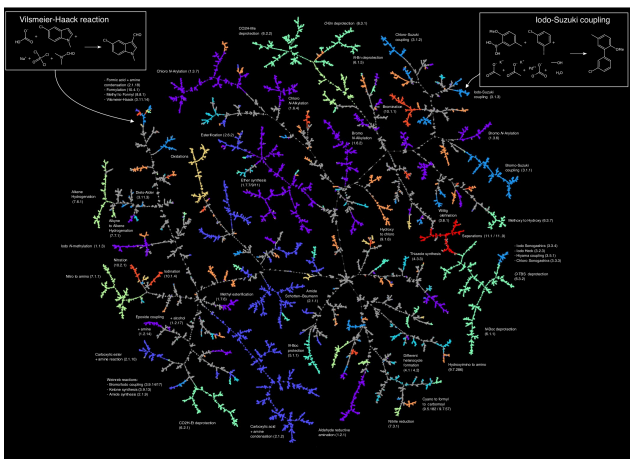

natural language processing

transformers

Schwaller, P., *et al.*, *Nat. Mach. Intell.*, 3: 144–152, 2021.

machine learning methods

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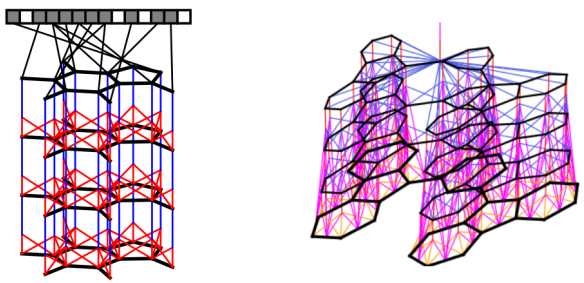

graph convolutions

Duvenaud, D., *et al.*, *NeurIPS 28*, 2015.

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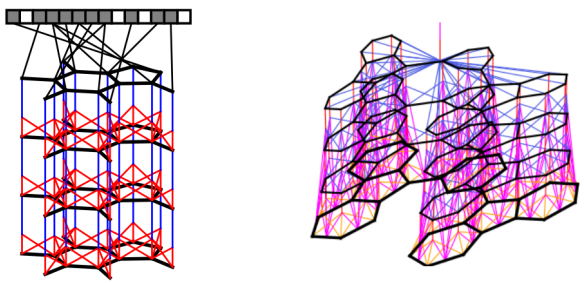

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diverse applications from traffic networks to medicine

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machine learning methods

Future directions for ML in chemistry

Some areas of high current interest:

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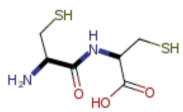
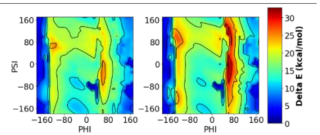
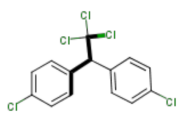
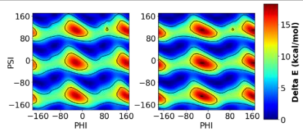
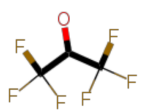
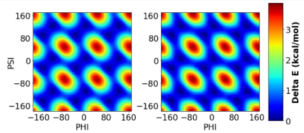
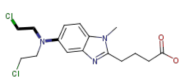
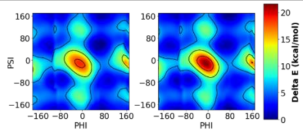
- Neural network potentials - quantum accuracy, force field cost. Reactive dynamics on your laptop!

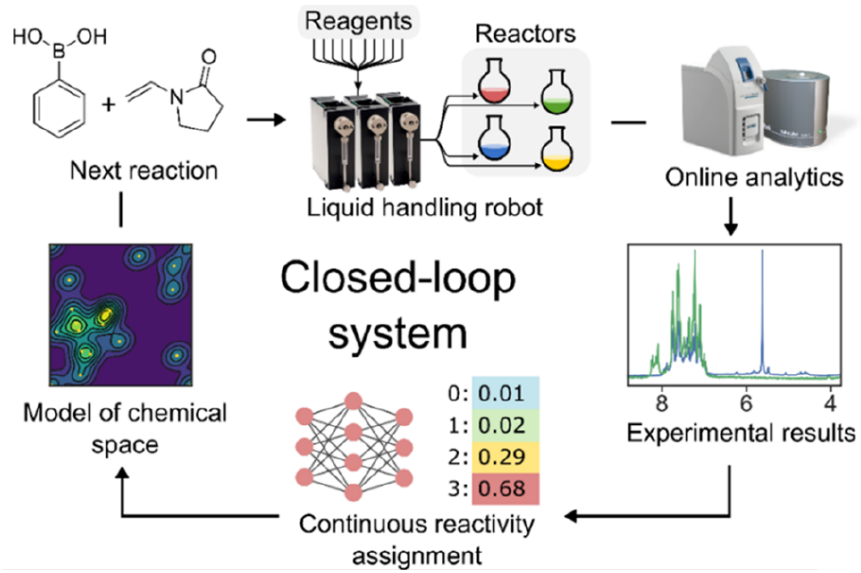
Name	Molecule	MAE	RMSE	Scan (Left:ANI Right:DFT)
Cysteine-Dipeptide (25 atoms)		1.75	2.55	
DDT (28 atoms)		0.53	0.70	
Hexafluoroacetone (10 atoms)		0.08	0.11	
Bendamustine (44 atoms)		0.50	0.66	

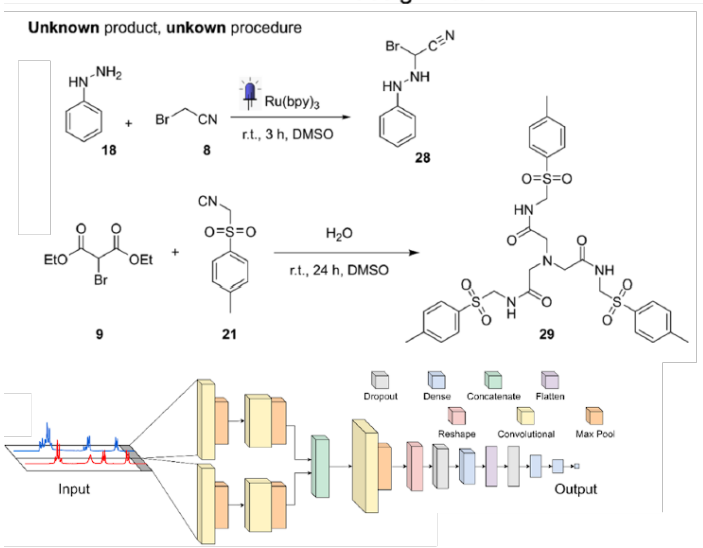
Devereux, C., *et al.*, *J. Chem. Theory Comput.*, 16(7):4192–4202, 2020

Future directions for ML in chemistry

Some areas of high current interest:

- Neural network potentials - quantum accuracy, force field cost. Reactive dynamics on your laptop!
- Synthesis planning and optimization. Fully automated chemistry!





Caramelli, D., *et al.*, *ACS Cent. Sci.*, just accepted, 2021

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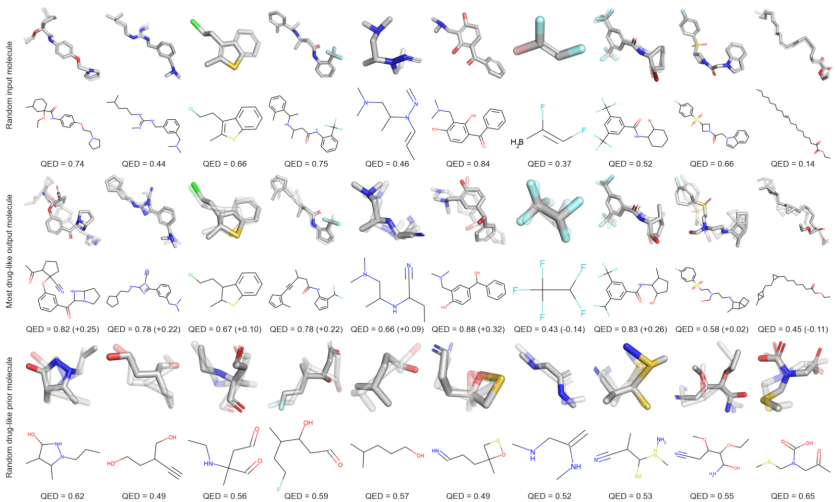
- Generative models. Designing new drugs directly into the pocket, *de novo*!



Ragoza, M., *et al.*, arXiv:2010.08687v3, 2020

Guo, J., *et al.*, *J .Cheminform.*, 13(89), 2021

Arcidiacono, M. & Koes, D.R., *et al.*, https://arxiv.org/abs/2109.15308, 2021

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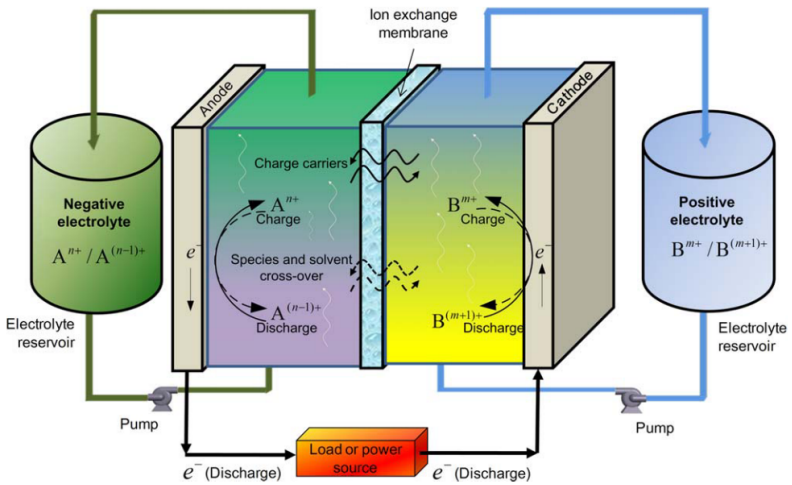

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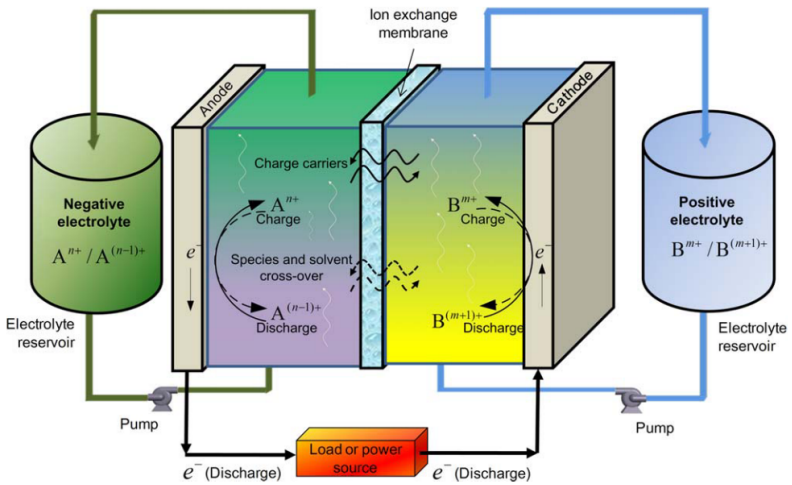

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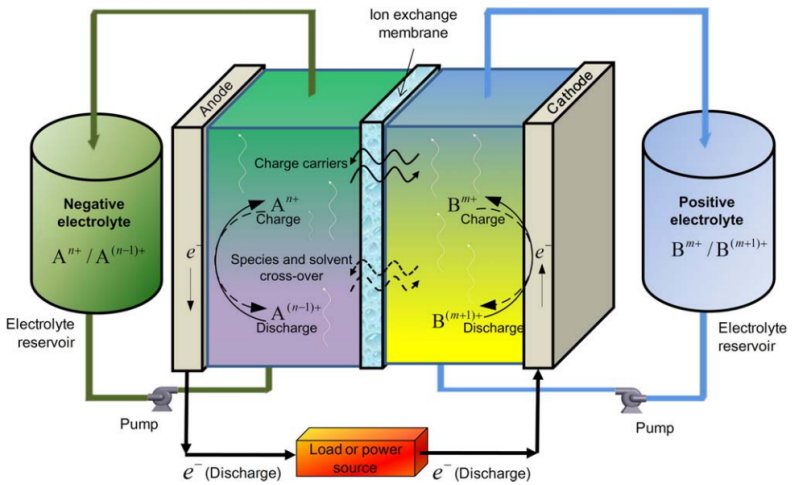

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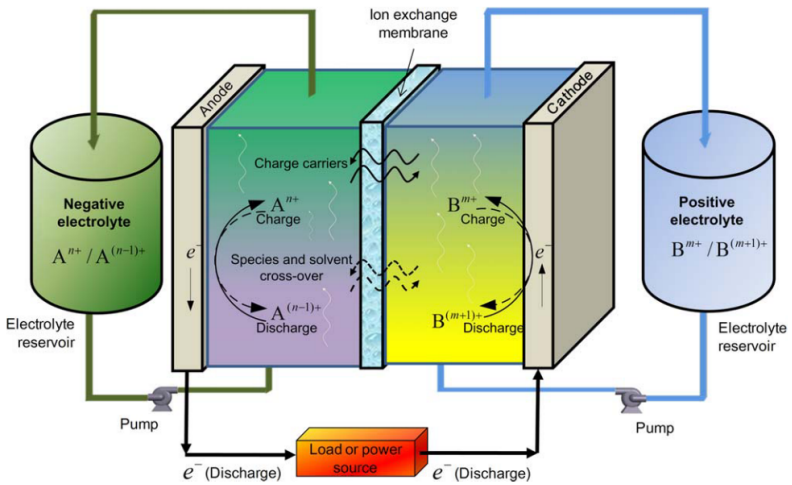

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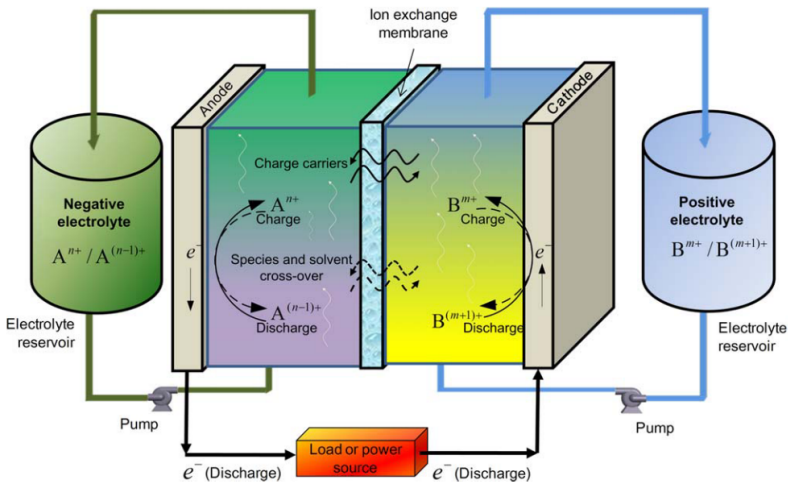

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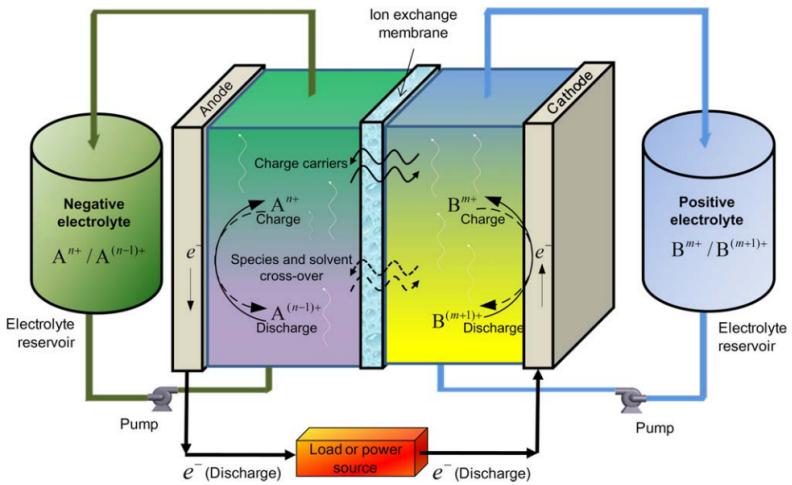

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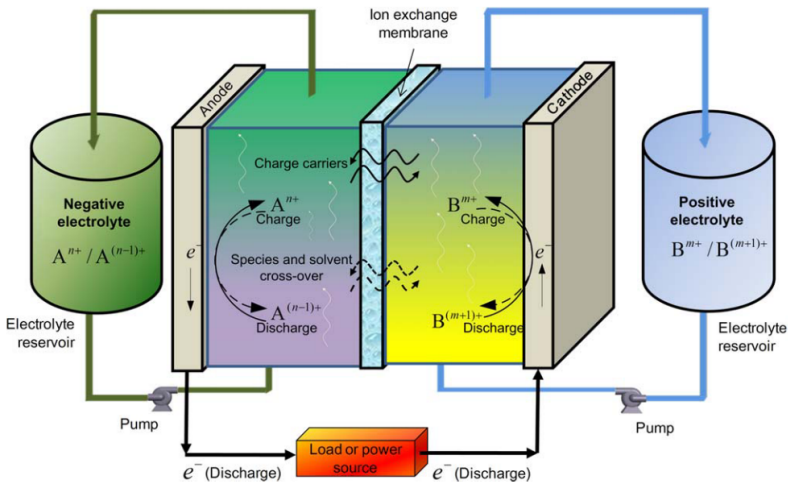

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We need complexes that have high redox potential **and** good solubility

A design space for RFBs

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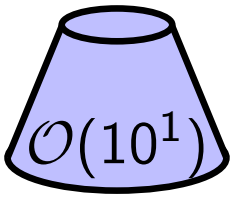

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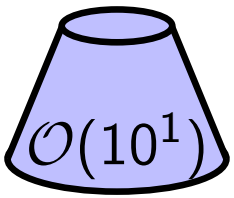

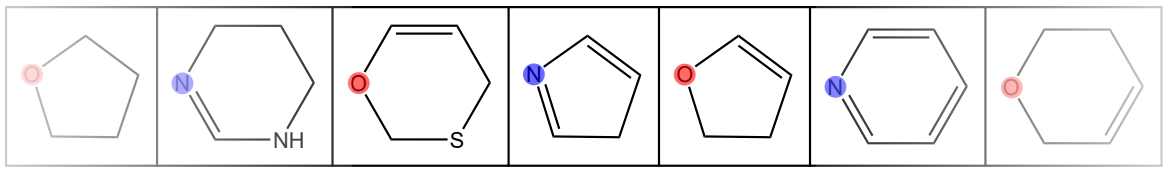

38 heterocycles

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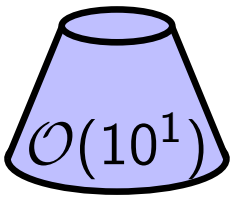

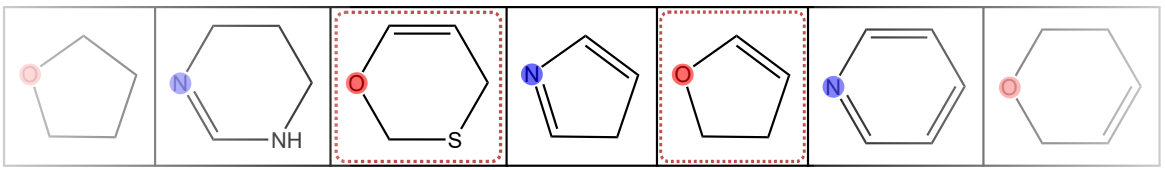

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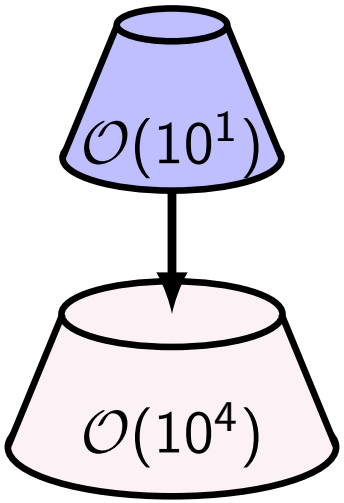
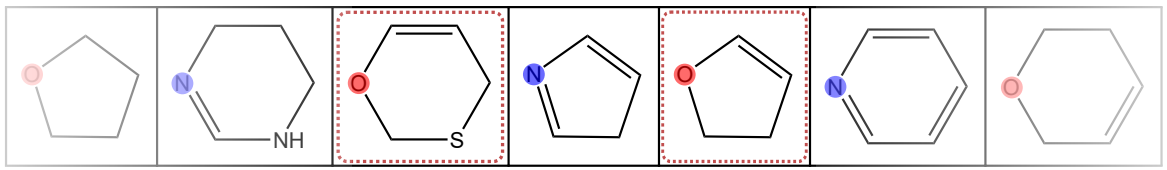
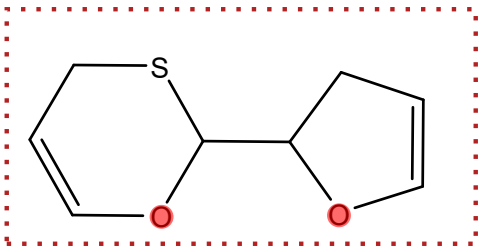
A design space for RFBs

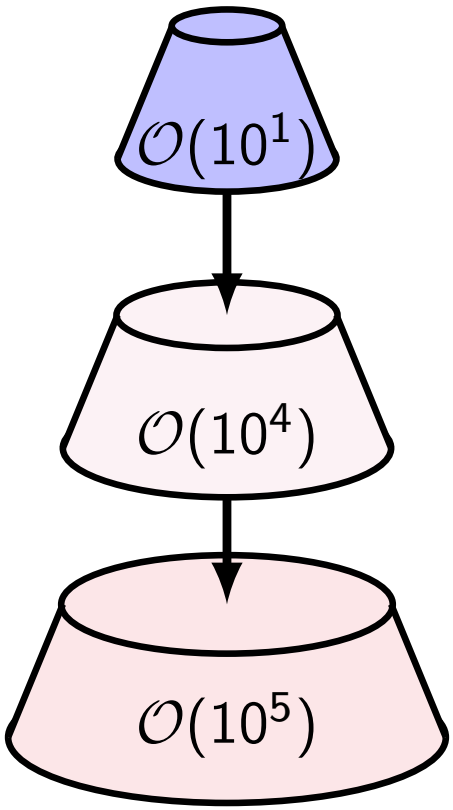


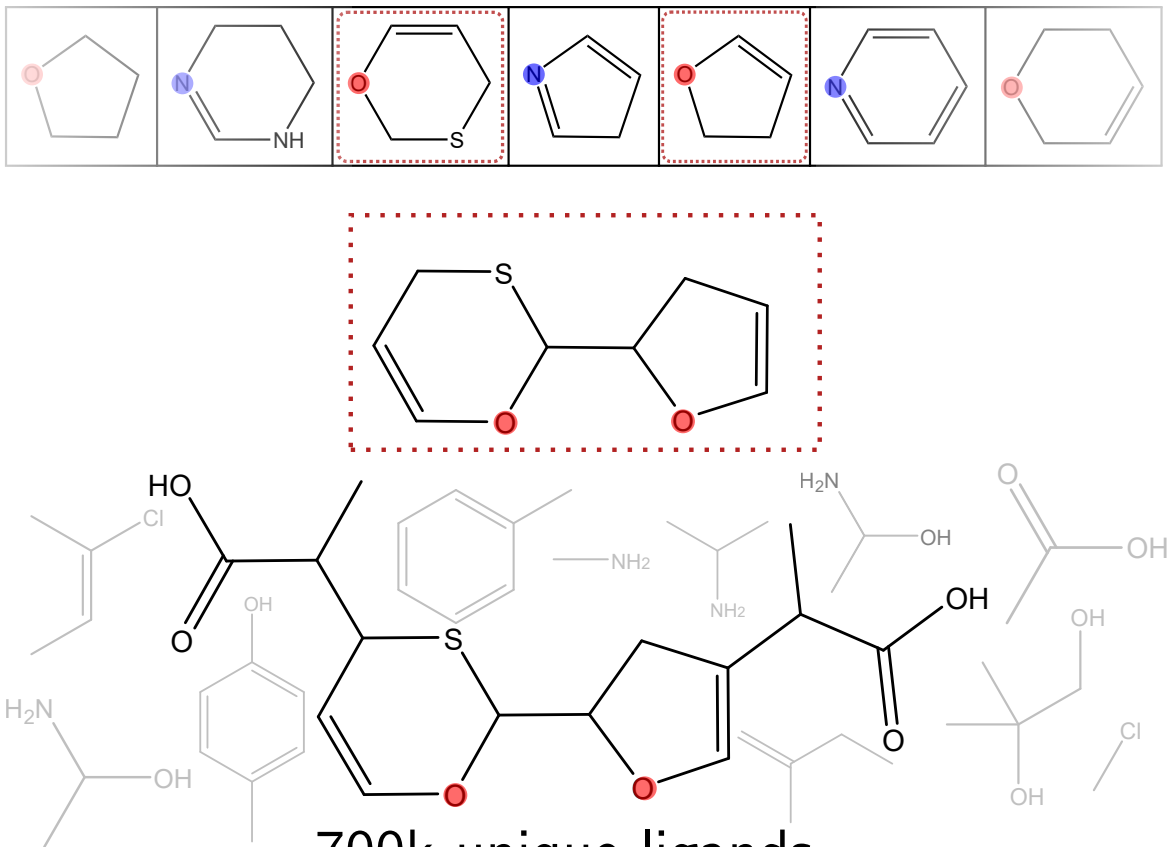




779 base ligands

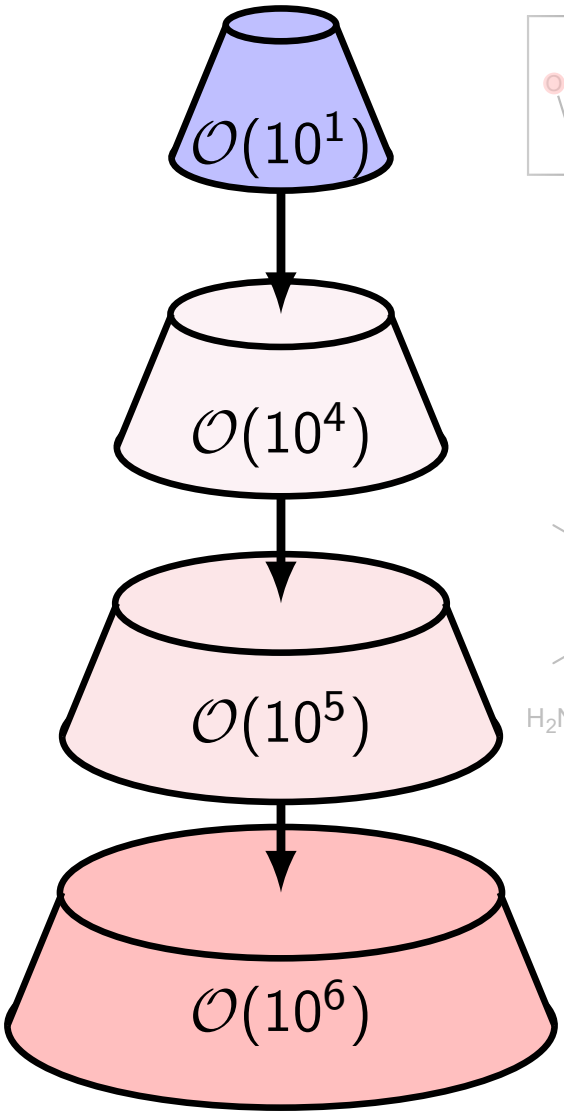
A design space for RFBs

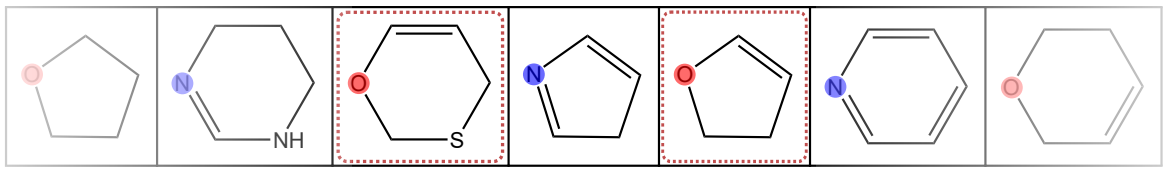


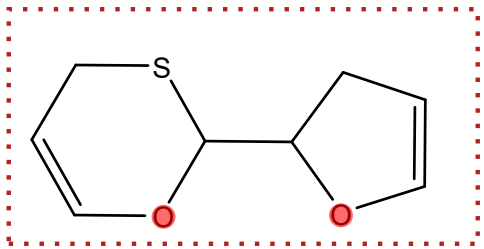


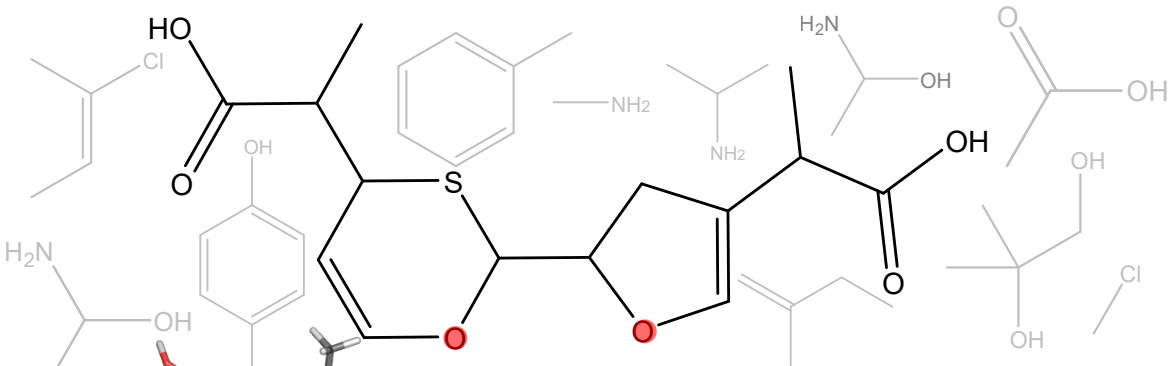
700k unique ligands

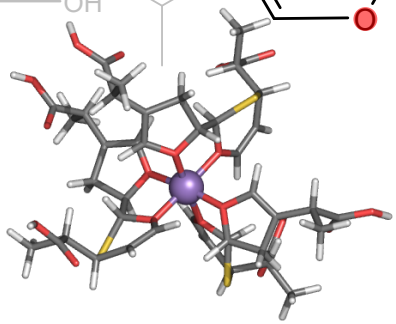
A design space for RFBs







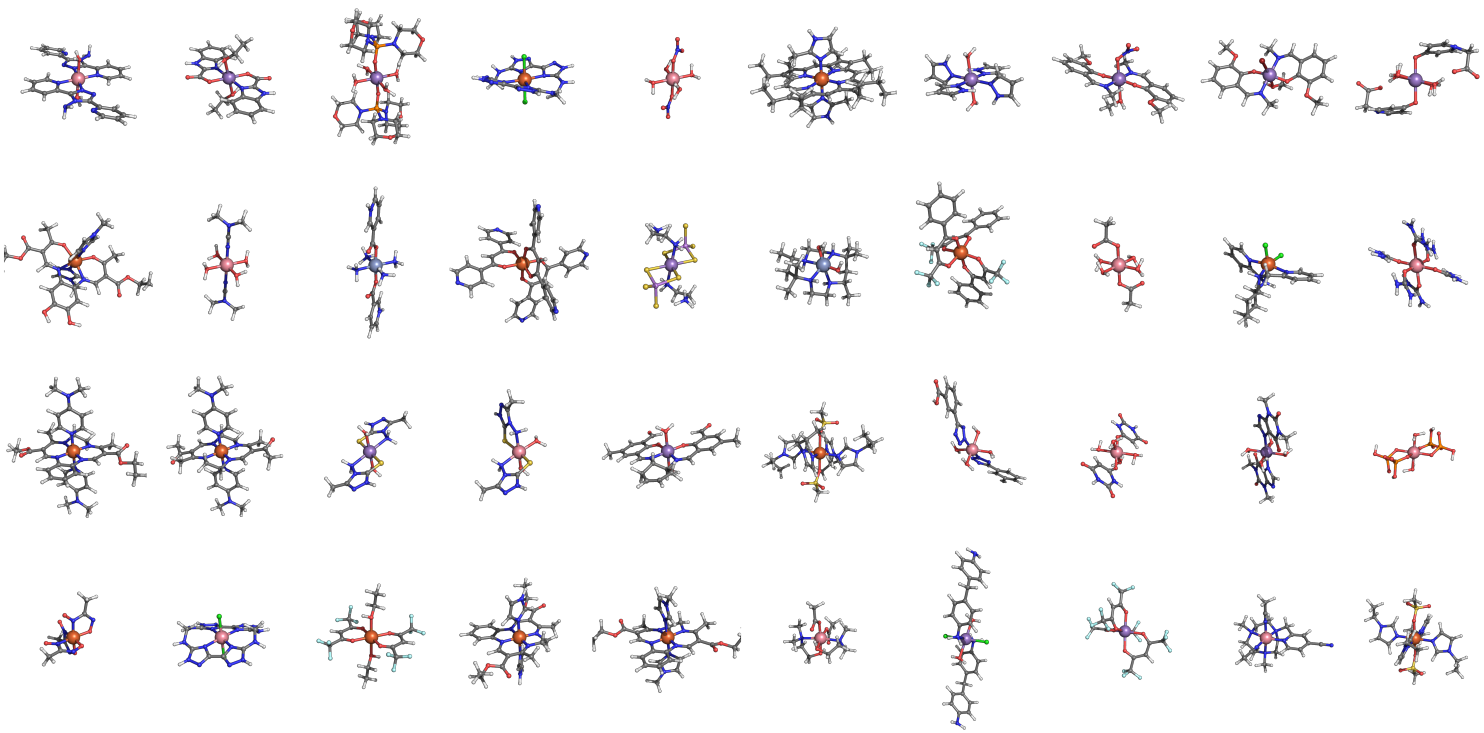




~ 3M complexes
with 4 metals

Computational approaches to chemical discovery

Computational methods can search for suitable complexes



Computational approaches to chemical discovery

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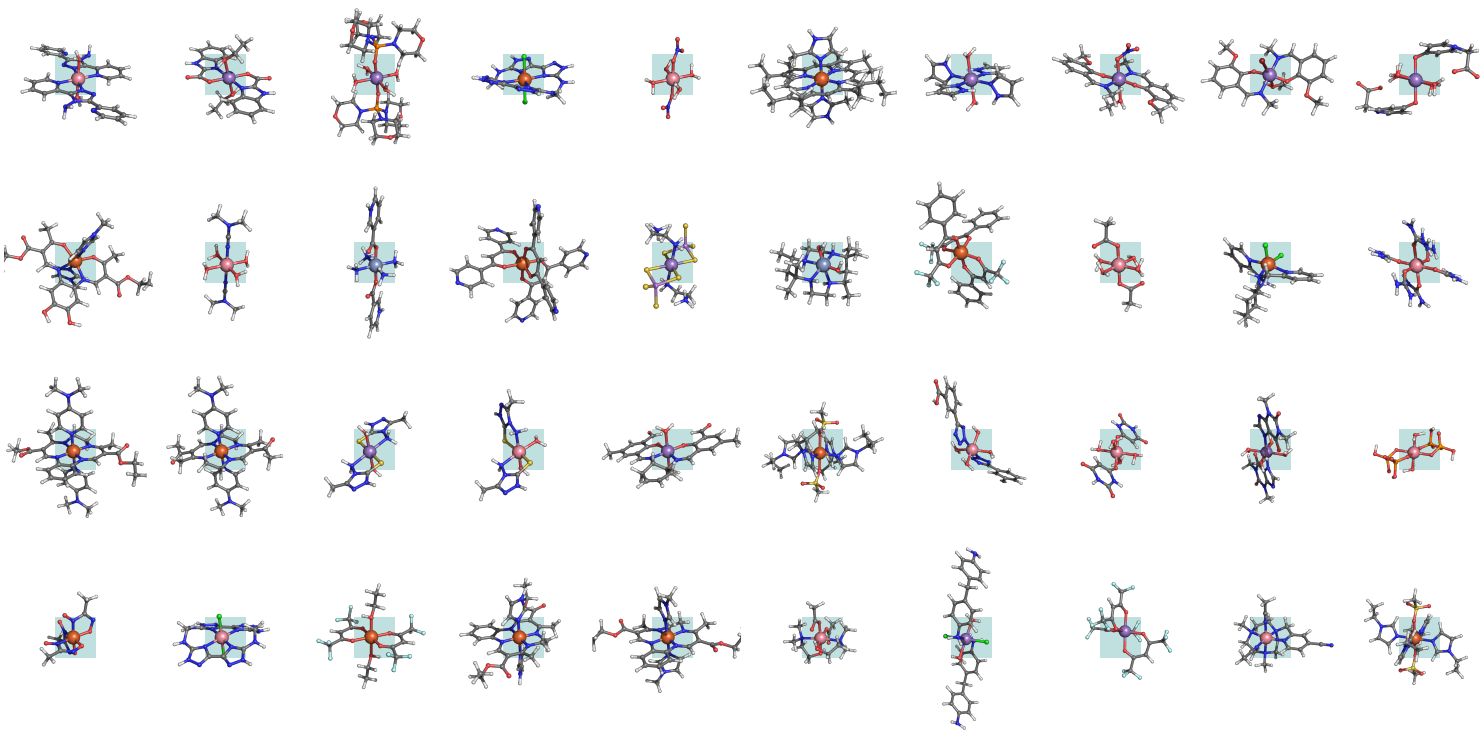

Computational approaches to chemical discovery

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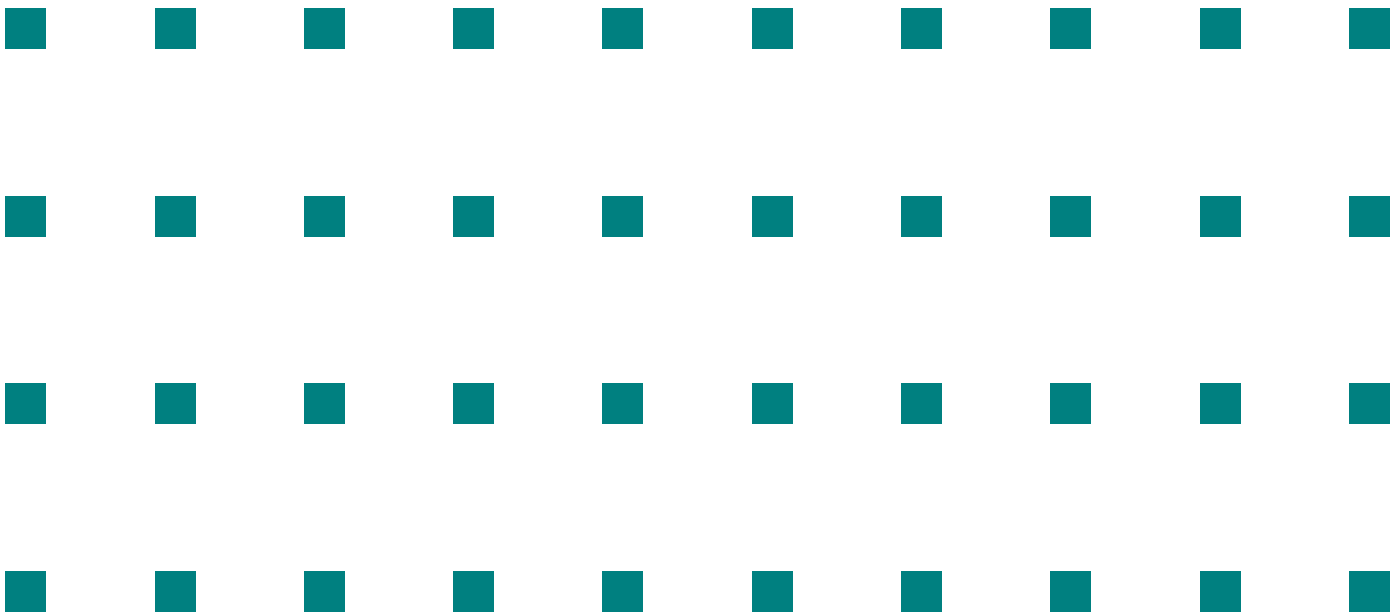

Computational approaches to chemical discovery

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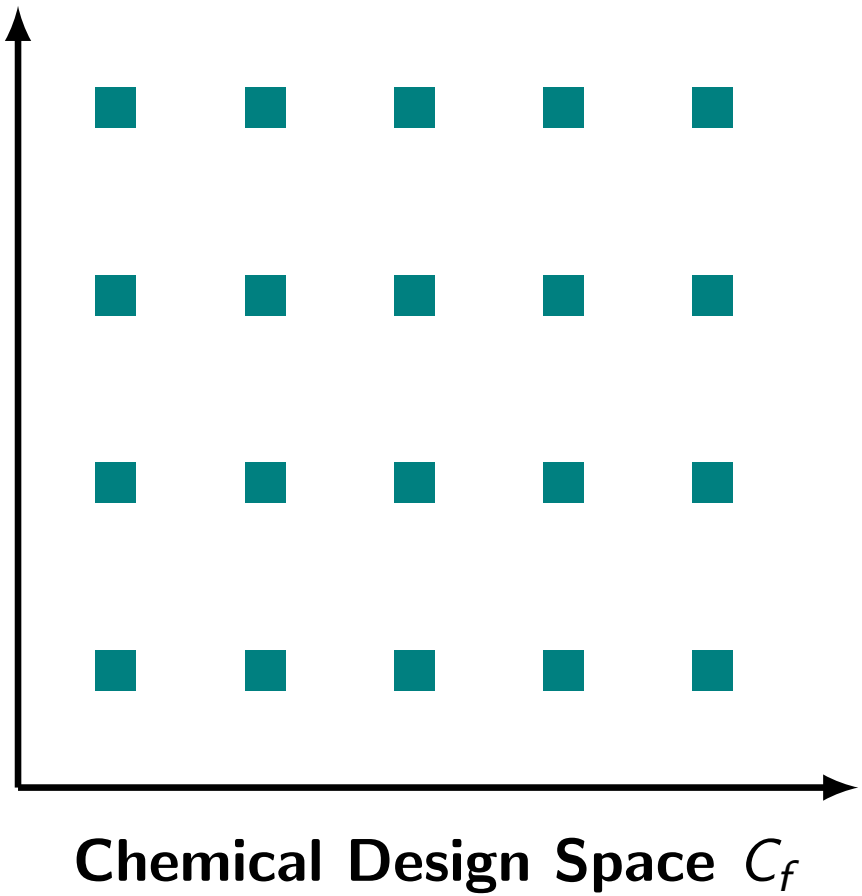
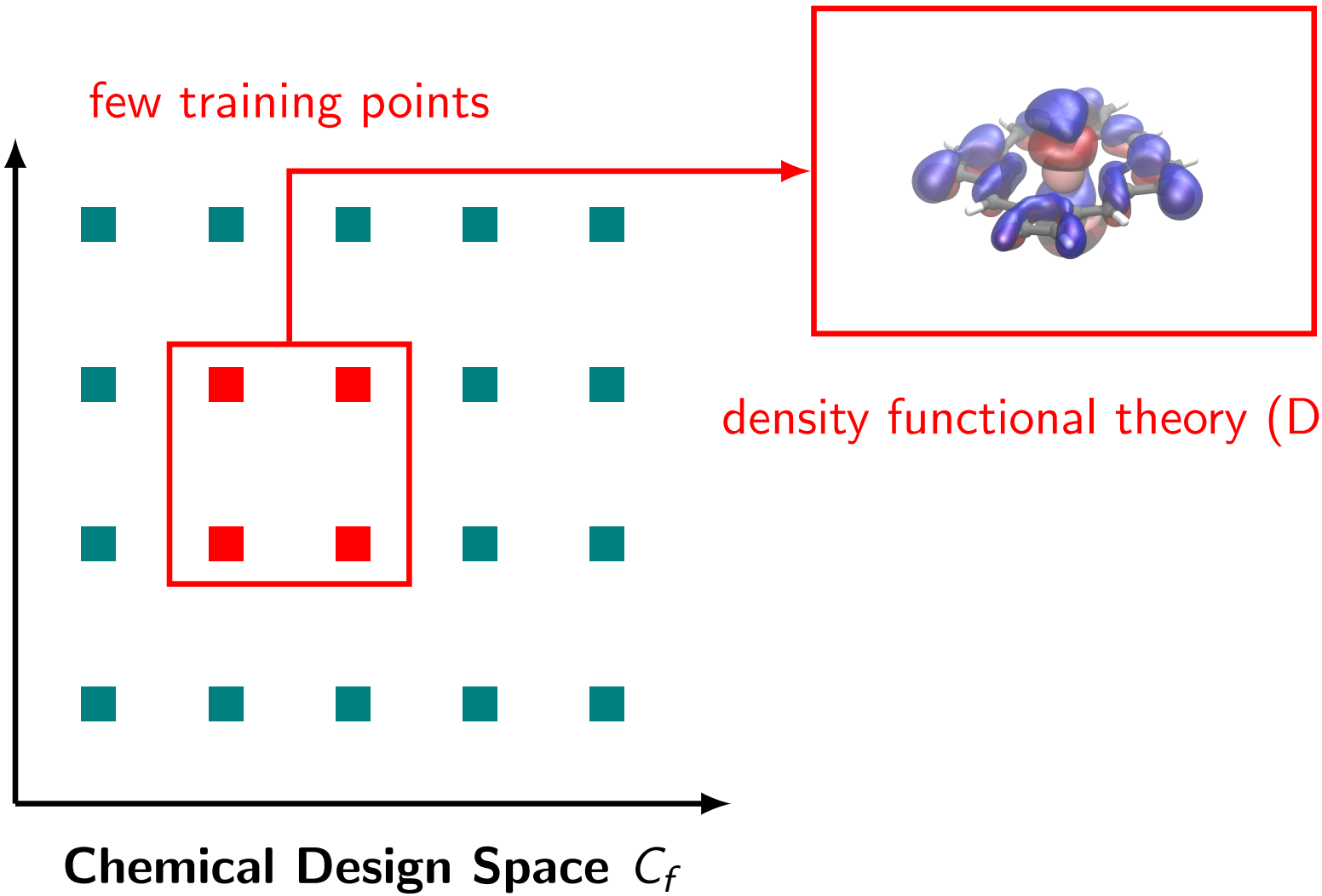
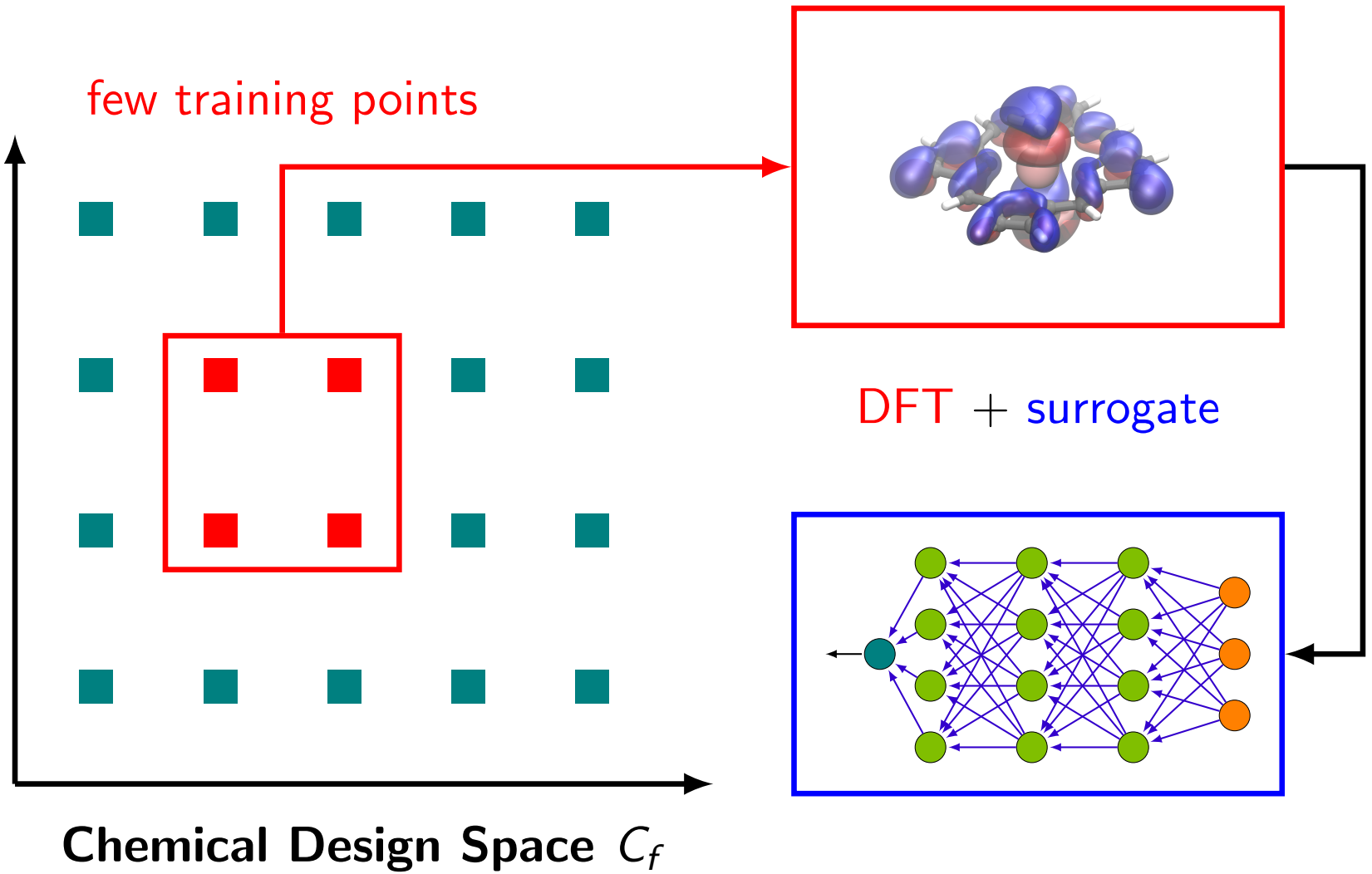


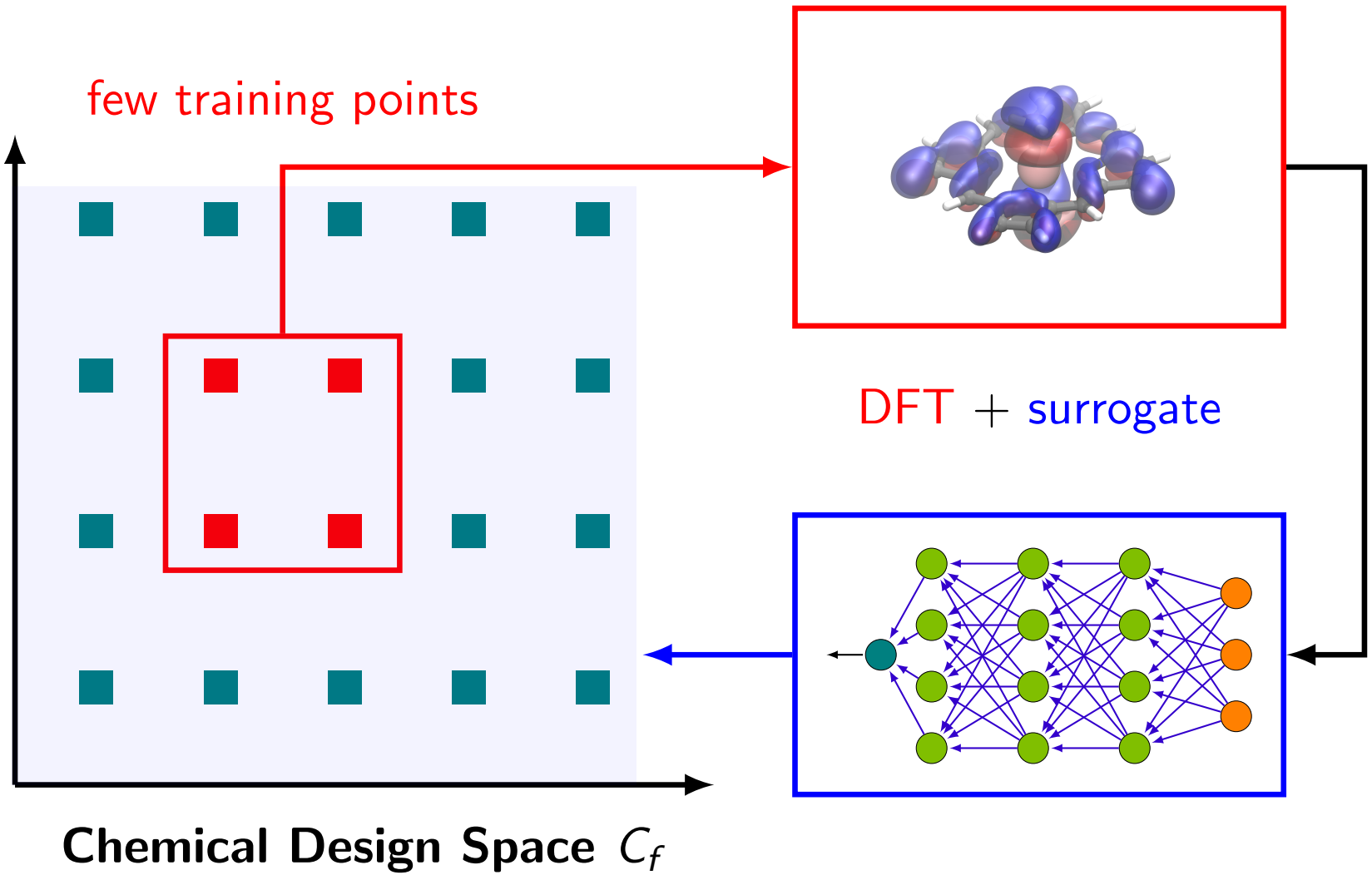
Computational approaches to chemical discovery



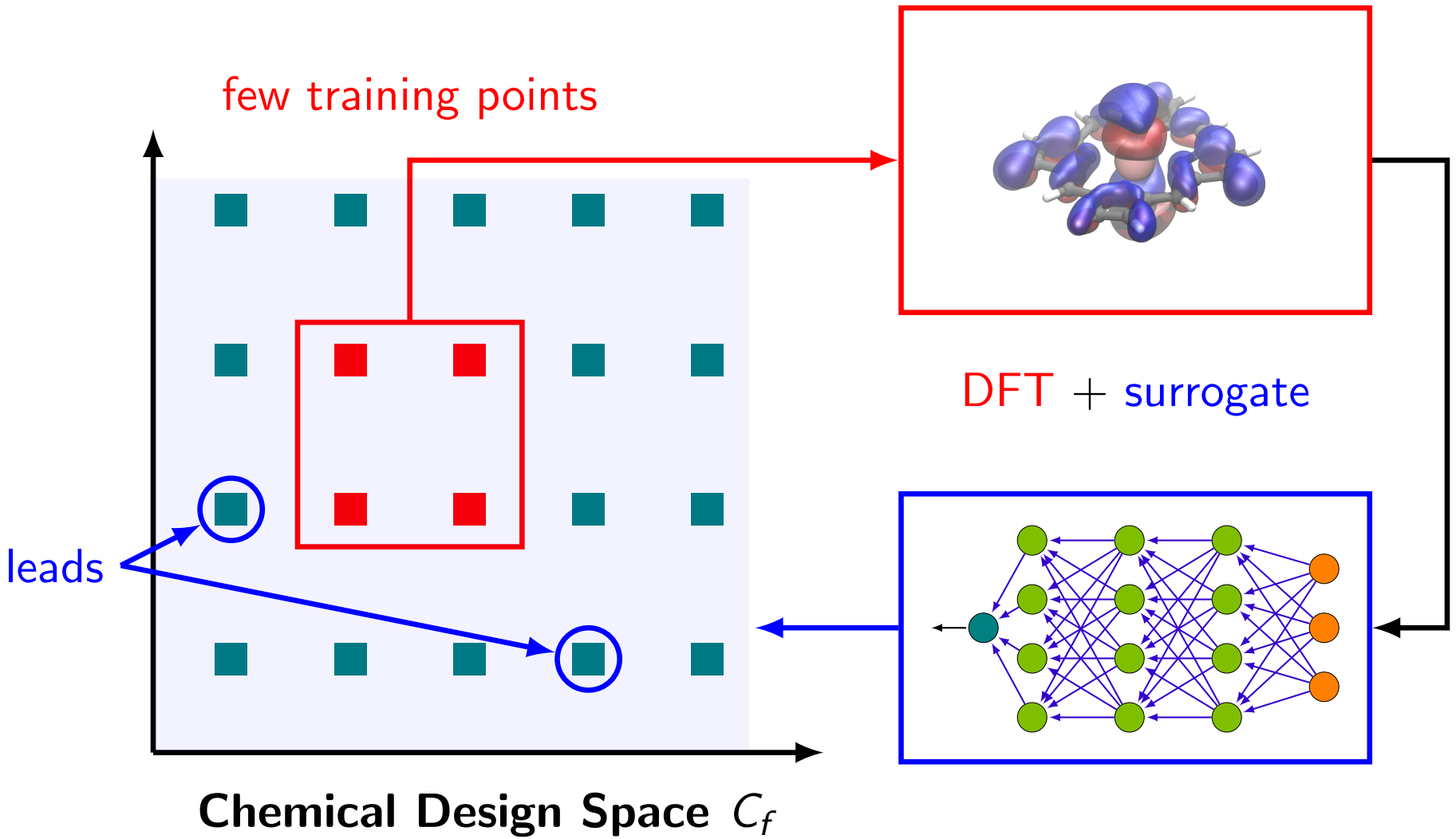
Computational approaches to chemical discovery



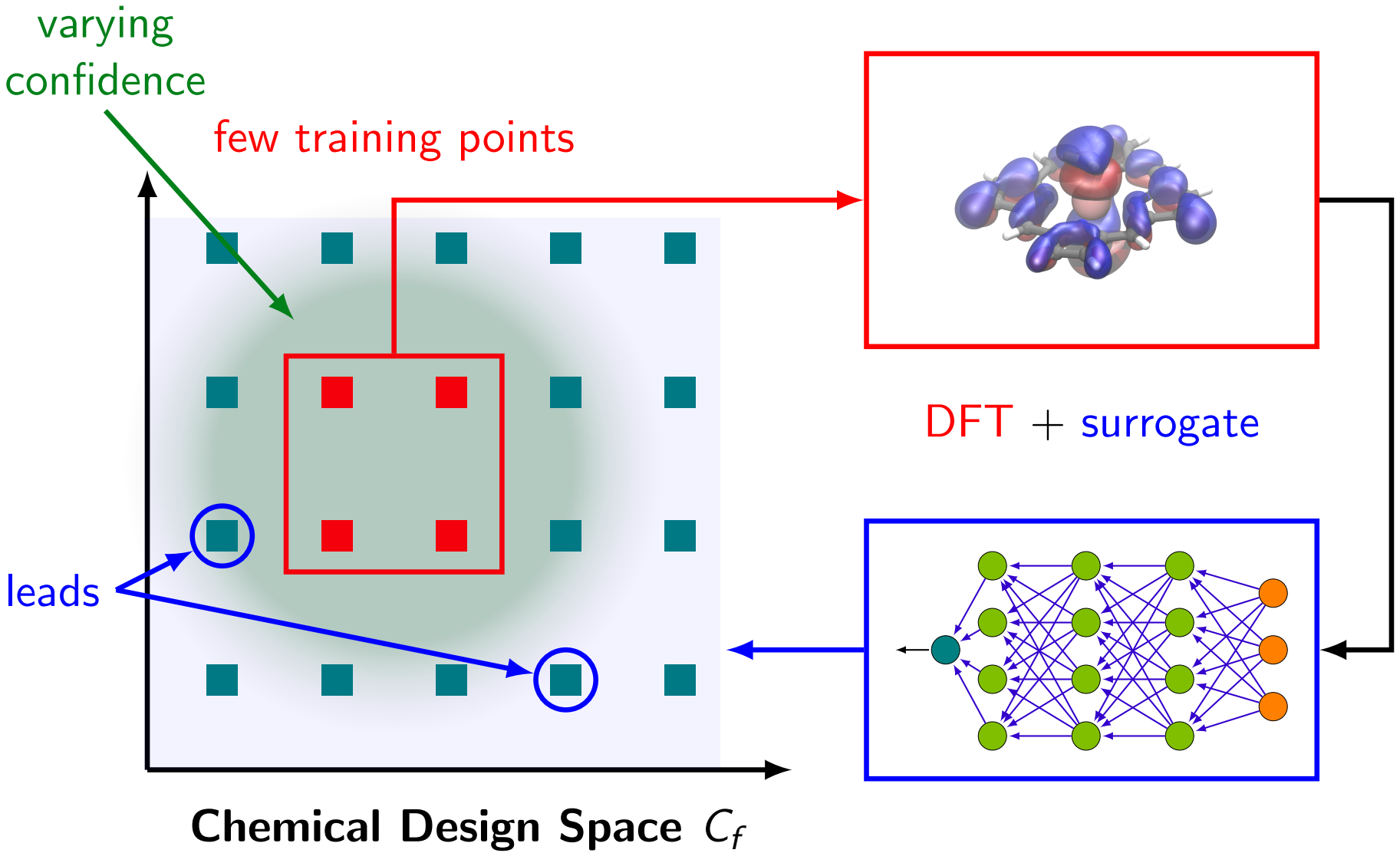
Computational approaches to chemical discovery



Computational approaches to chemical discovery



Computational approaches to chemical discovery



Multiobjective optimization

We can predict quantites of interest for our RFBs with ANNs

Janet, J.P., *et al.*, *ACS Cent. Sci.*, 6(4):513–524, 2020

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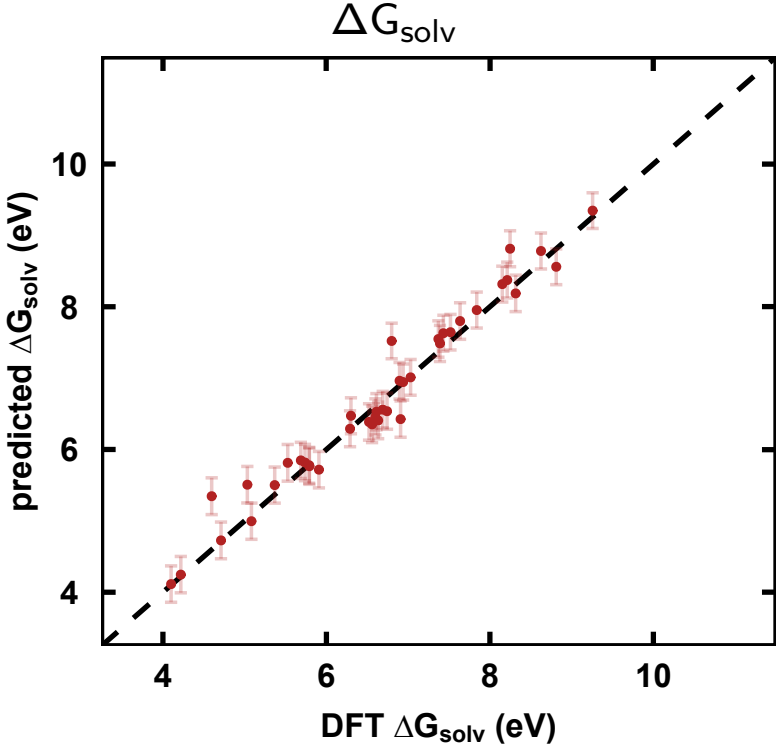

Janet, J.P., *et al.*, *ACS Cent. Sci.*, 6(4):513–524, 2020

3 × 100 tanh nodes, multitask, fully connected

Multiobjective optimization

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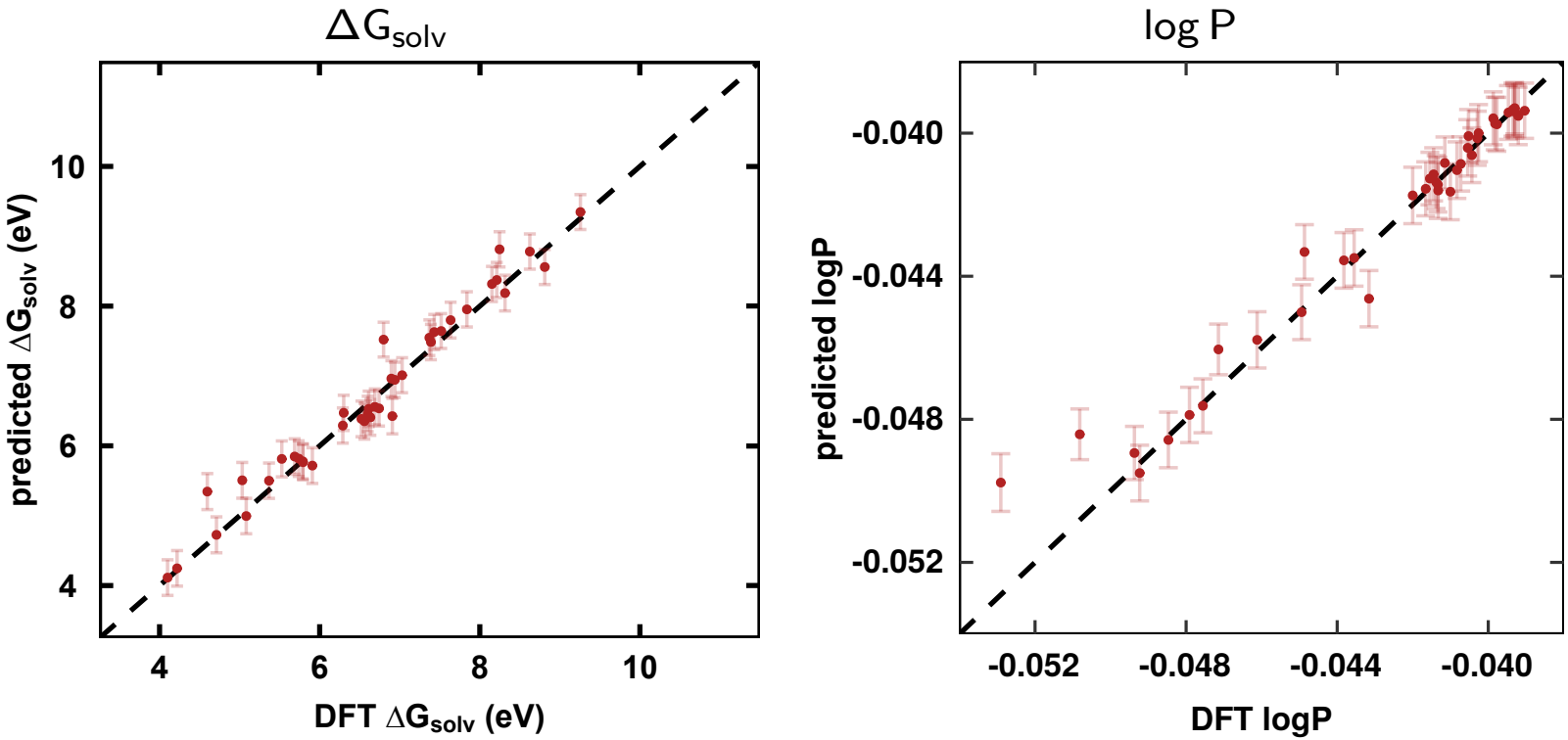

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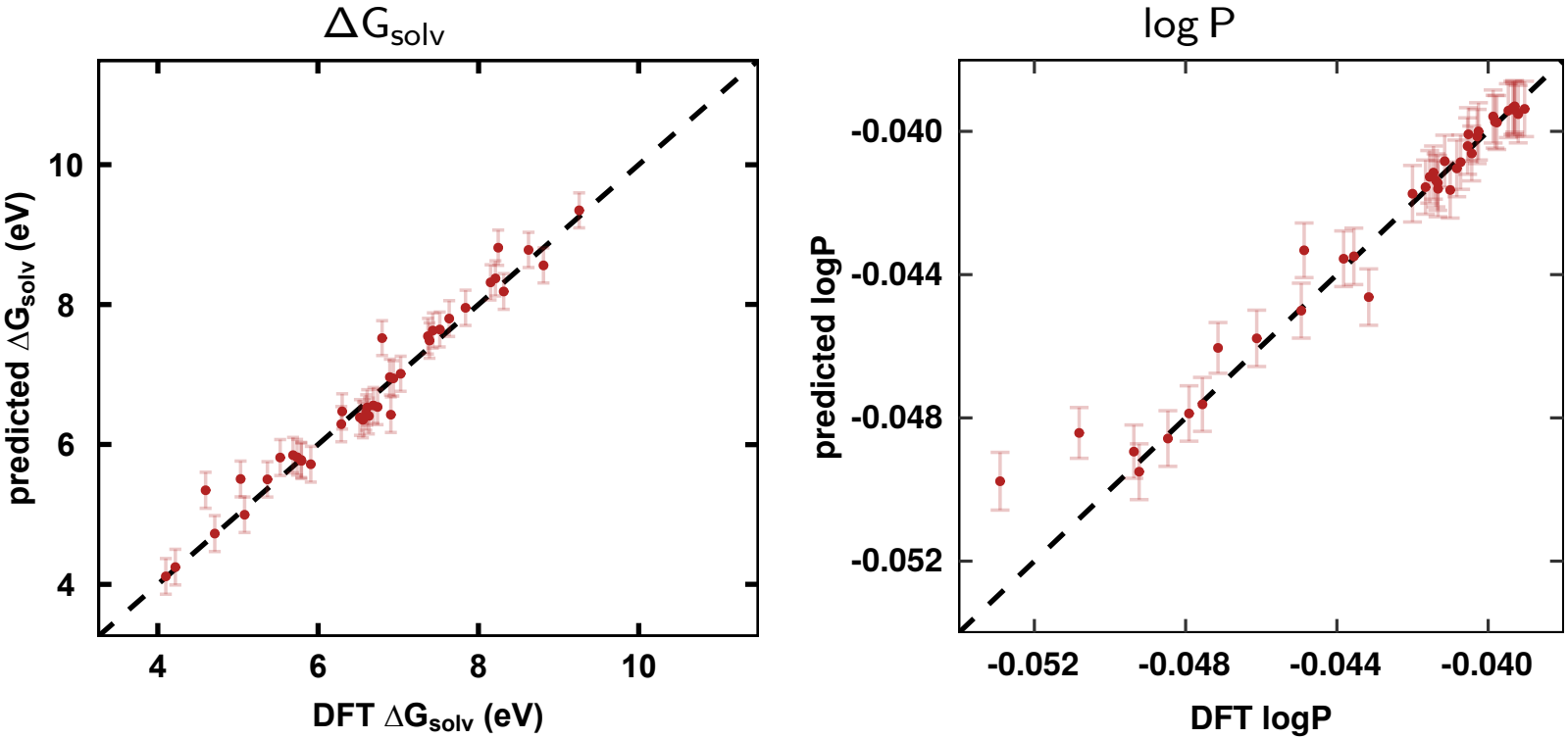

Screen $3M$ complexes in < 4 **minutes** on a regular workstation, c.f. 50 **GPU-years** with DFT

Janet, J.P., *et al.*, *ACS Cent. Sci.*, 6(4):513–524, 2020

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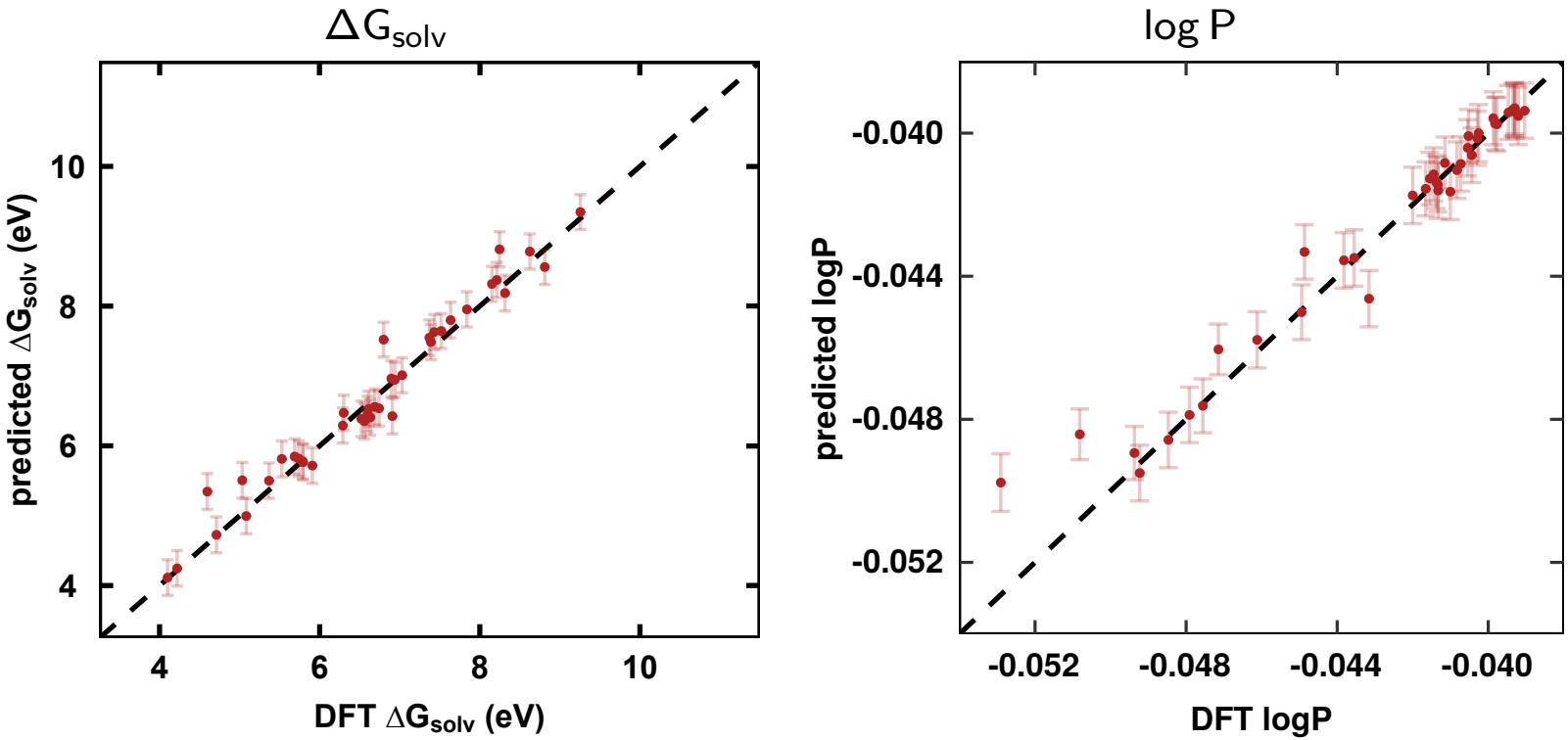

$$\begin{matrix}\Delta G_{solv} \\ \log P\end{matrix} = \begin{bmatrix}\hat{y}_1 \\ \hat{y}_2\end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix}\hat{\mu}_1 \\ \hat{\mu}_2\end{bmatrix}, \begin{bmatrix}\hat{\sigma}_1^2 & 0 \\ 0 & \hat{\sigma}_2^2\end{bmatrix}\right)$$

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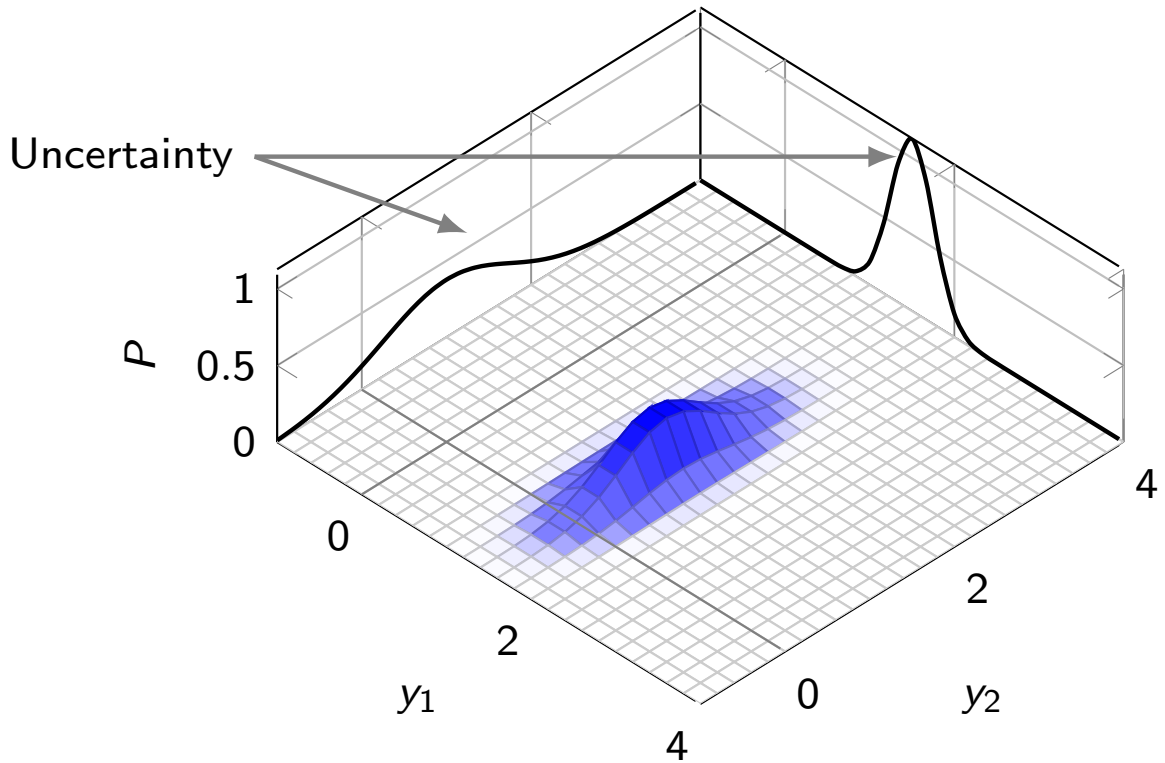

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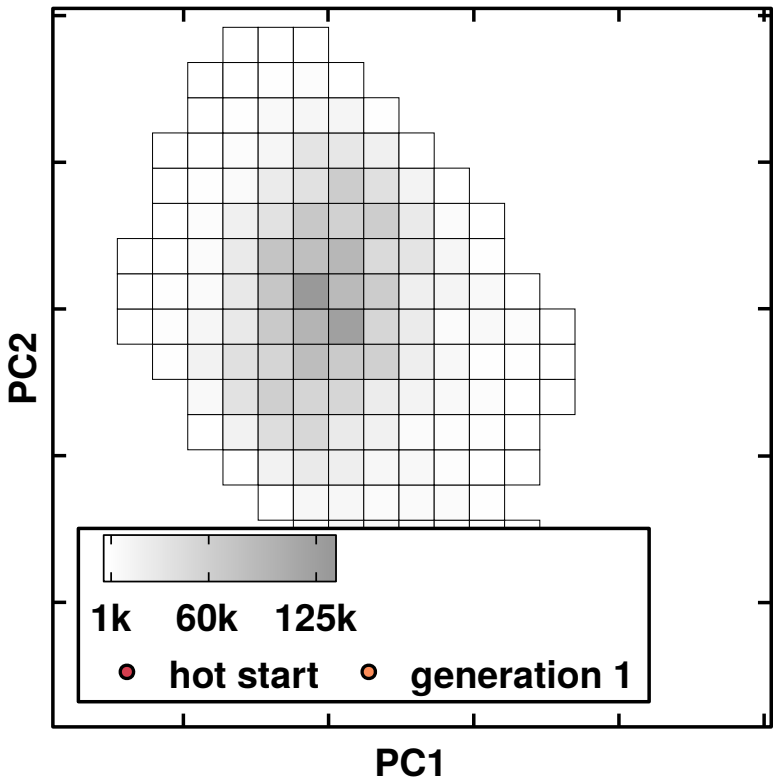
Janet, J.P., *et al.*, *ACS Cent. Sci.*, 6(4):513–524, 2020

3×100 tanh nodes, multitask, fully connected

Design space and clustering

Jump start the design with diversity-oriented cluster:



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Design space and clustering

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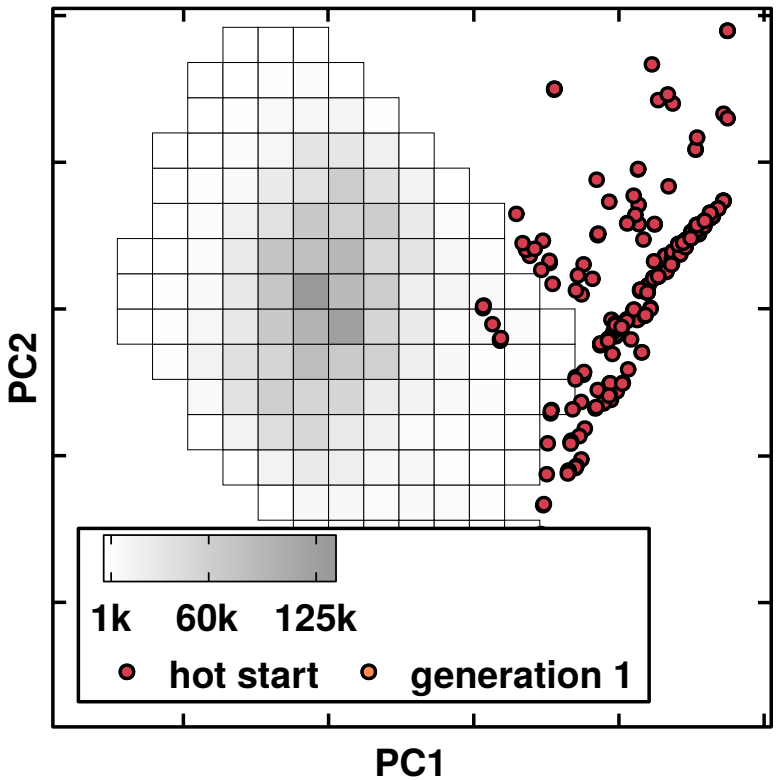

Janet, J.P., *et al.*, *ACS Cent. Sci.*, 6(4):513–524, 2020

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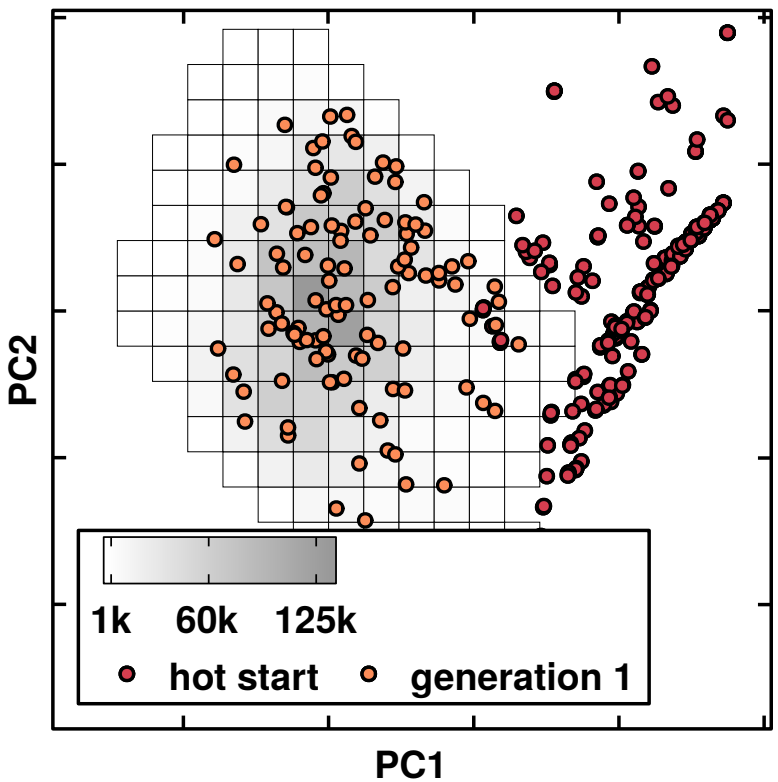

design space

Janet, J.P., *et al.*, *ACS Cent. Sci.*, 6(4):513–524, 2020

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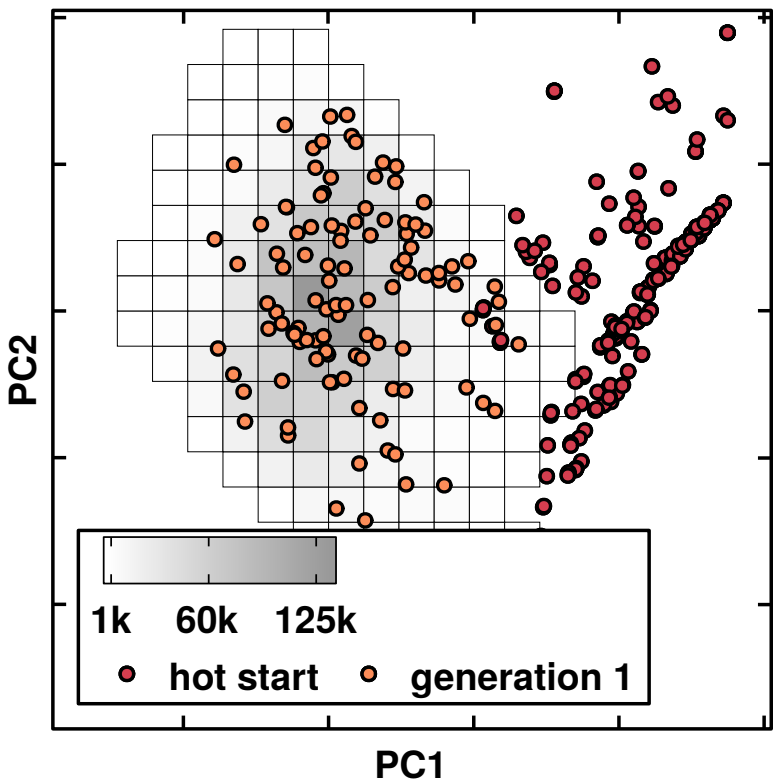

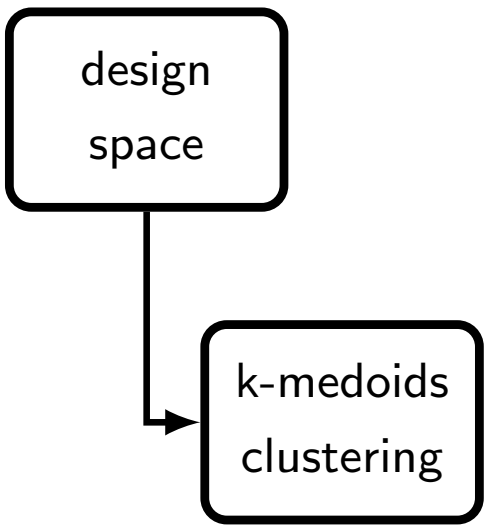

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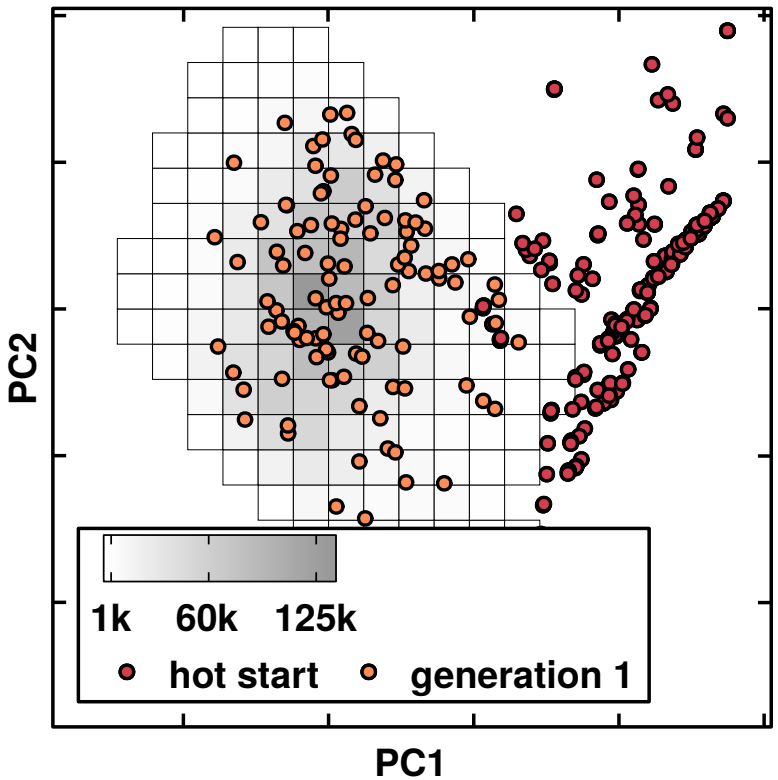

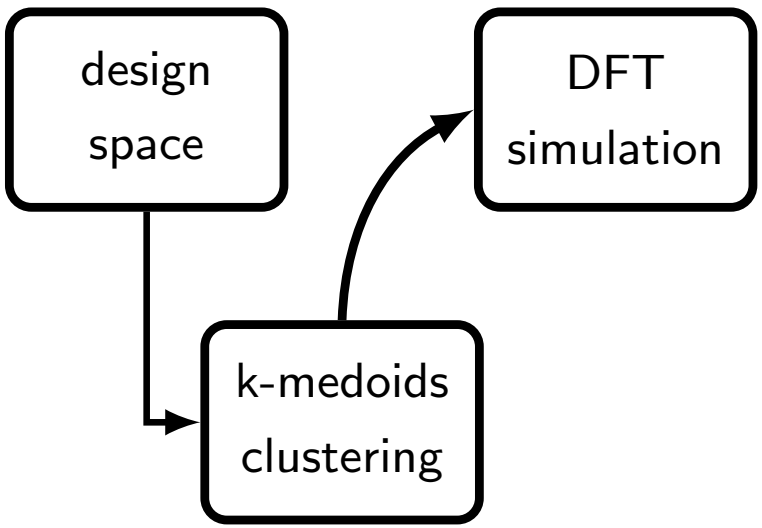

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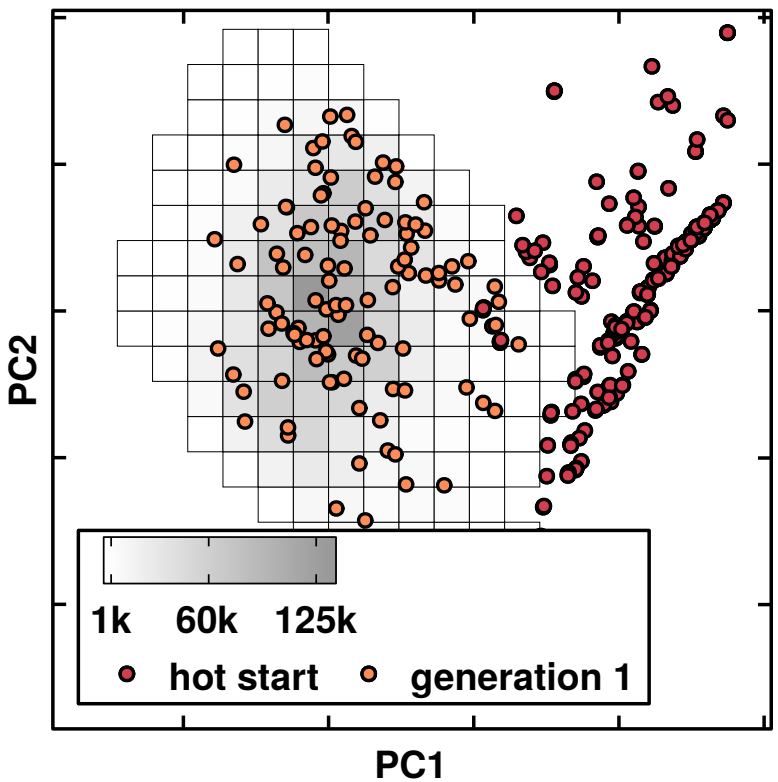

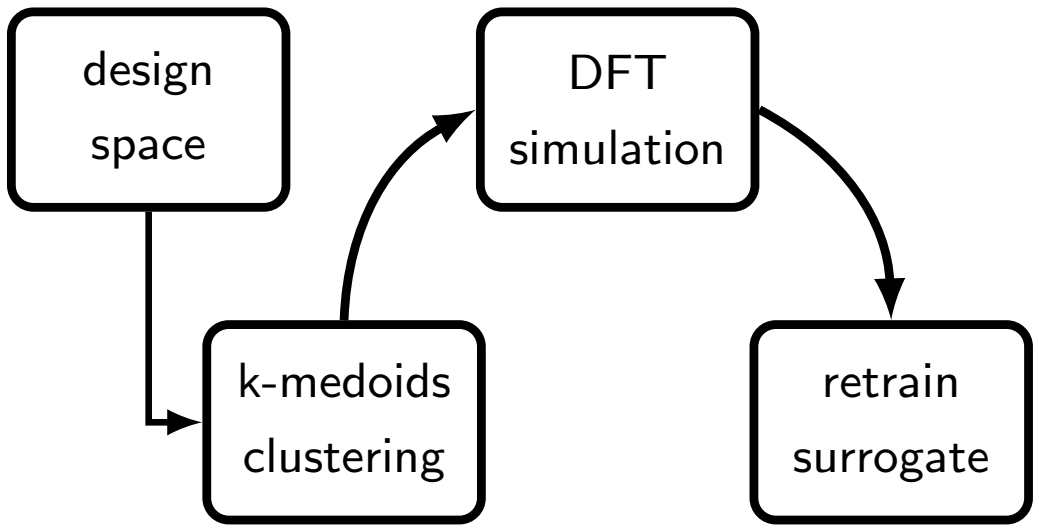

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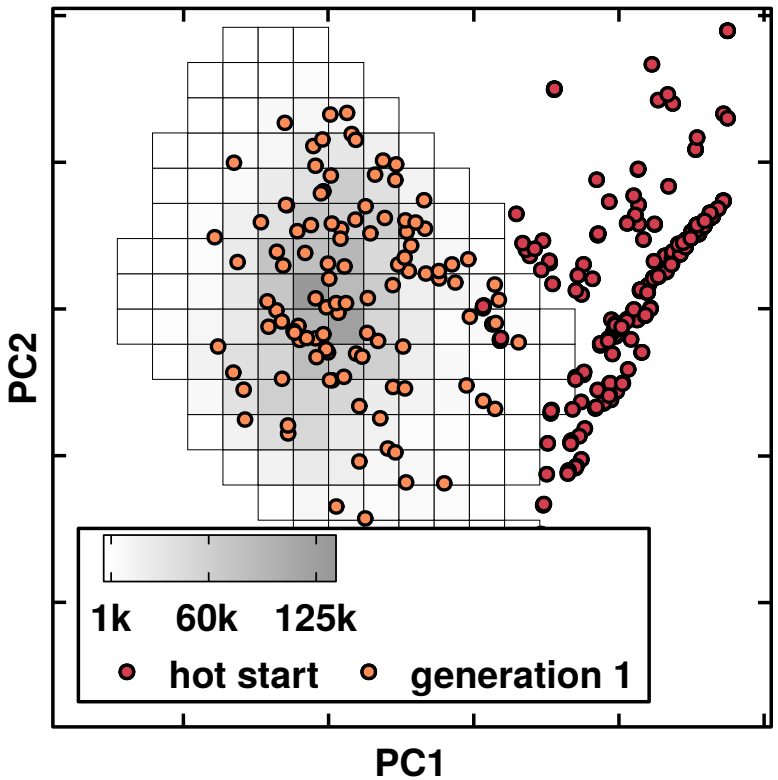

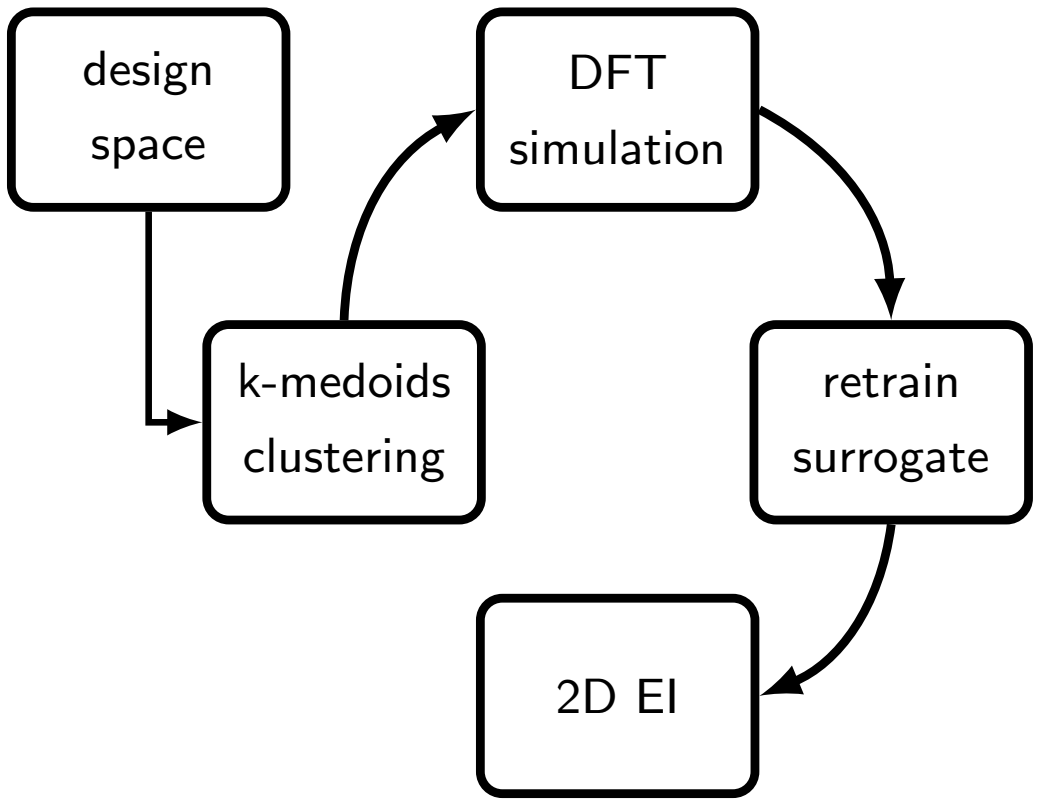

Janet, J.P., *et al.*, *ACS Cent. Sci.*, 6(4):513–524, 2020

multitask: 2 × 100 tanh nodes, fully connected

Design space and clustering

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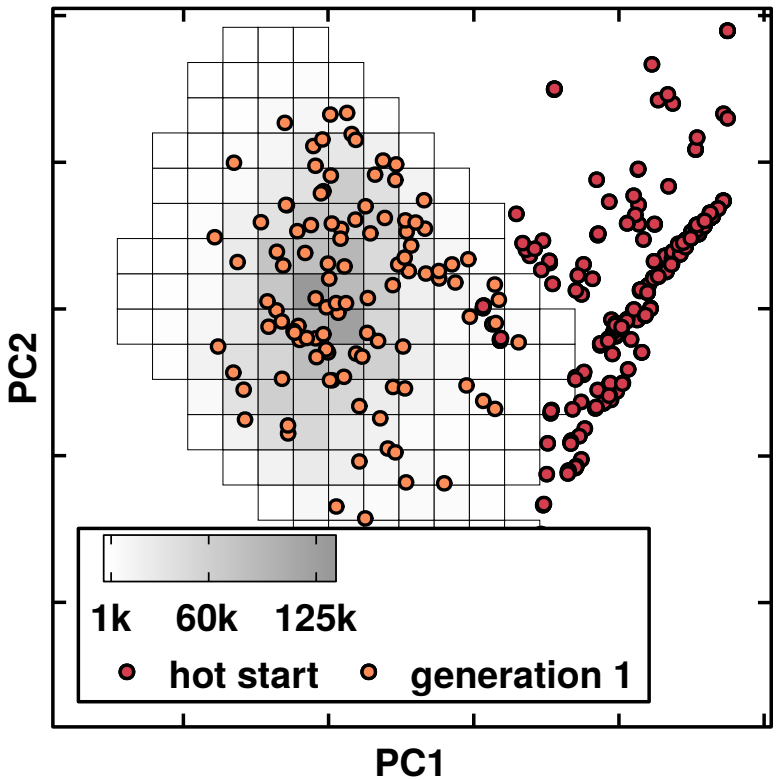
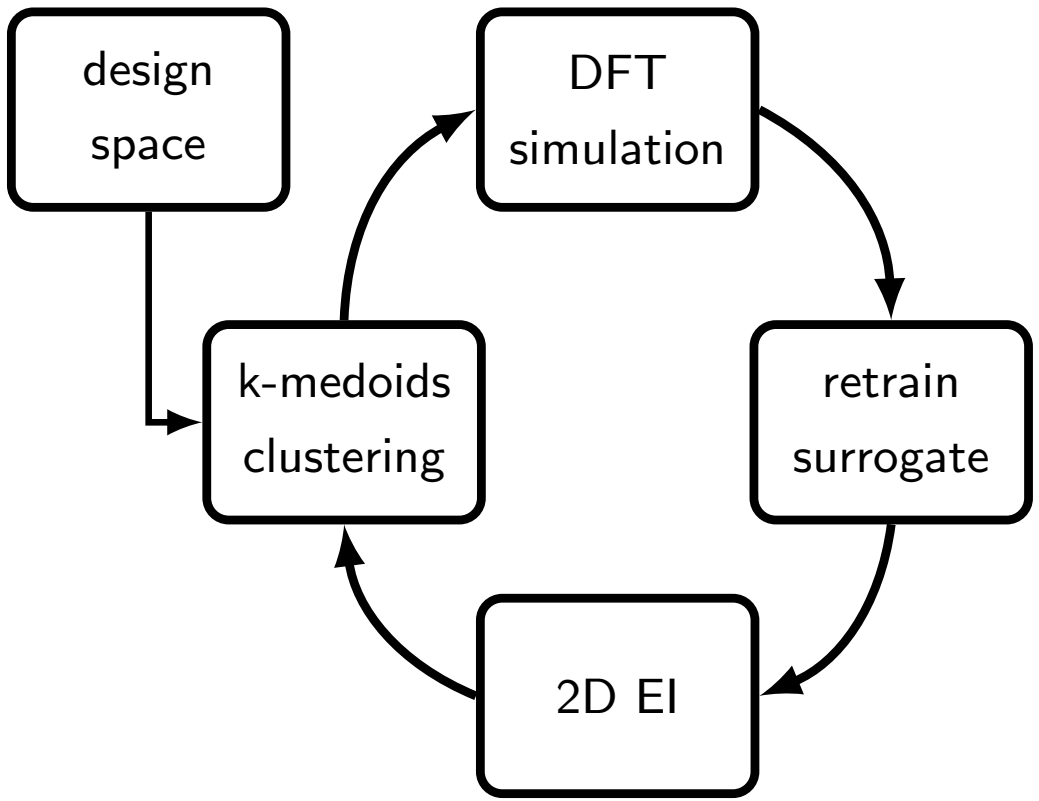


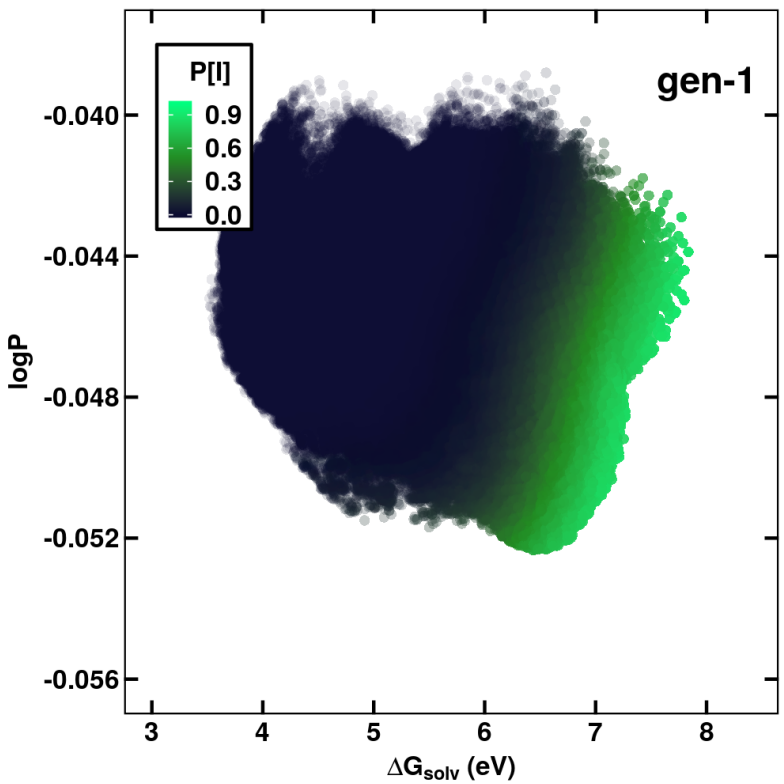


Janet, J.P., *et al.*, *ACS Cent. Sci.*, 6(4):513–524, 2020

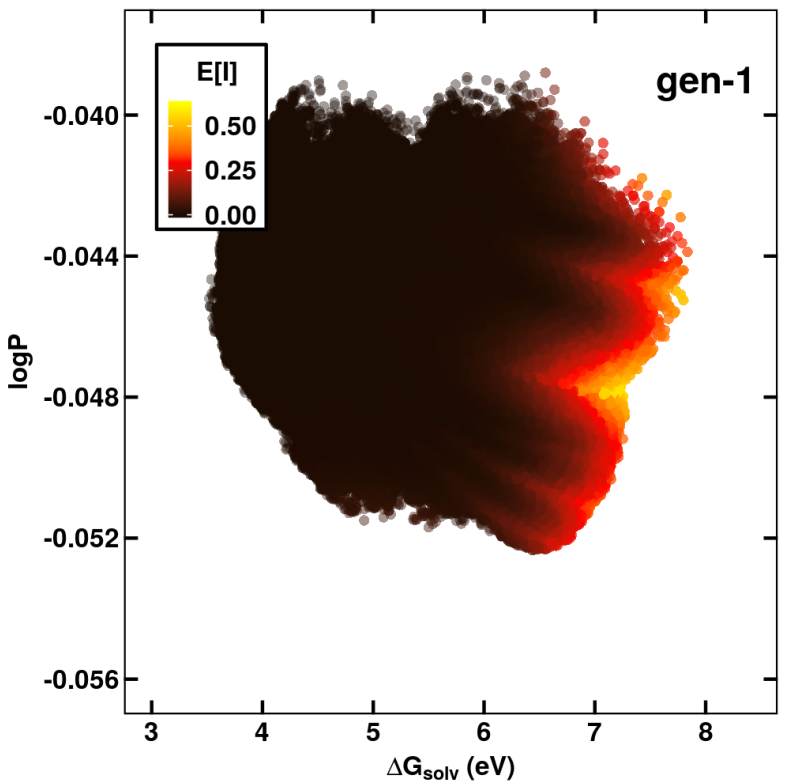
multitask: 2 × 100 tanh nodes, fully connected

Evolution of PI and EI

probability of improvement



expected improvement



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Evolution of PI and EI

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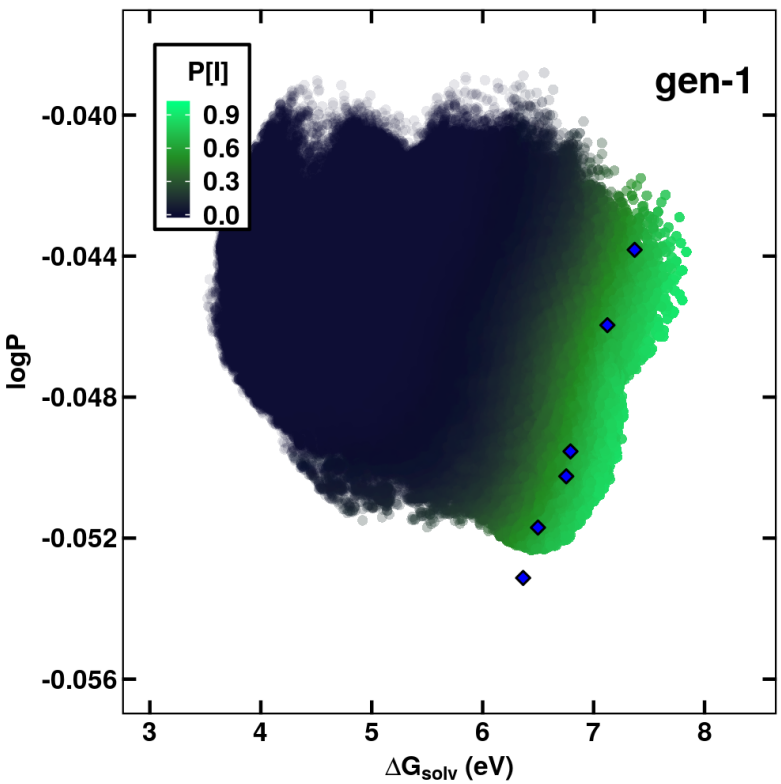

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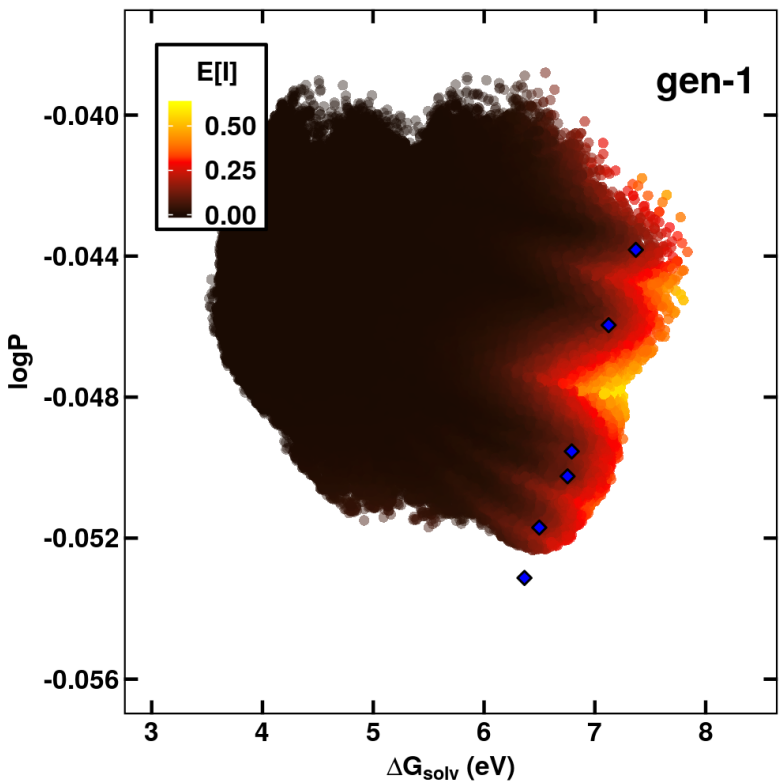

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Evolution of PI and EI

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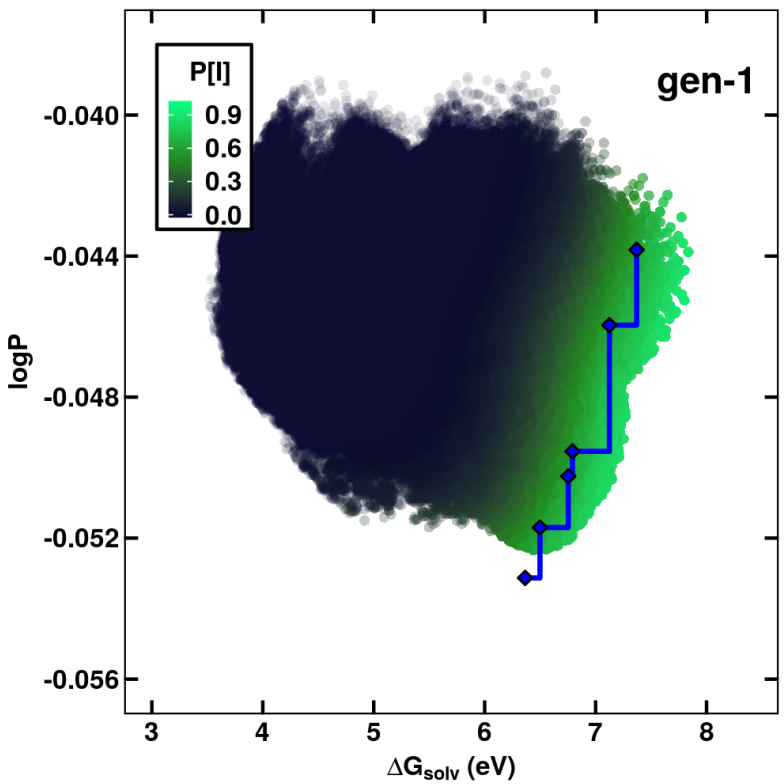

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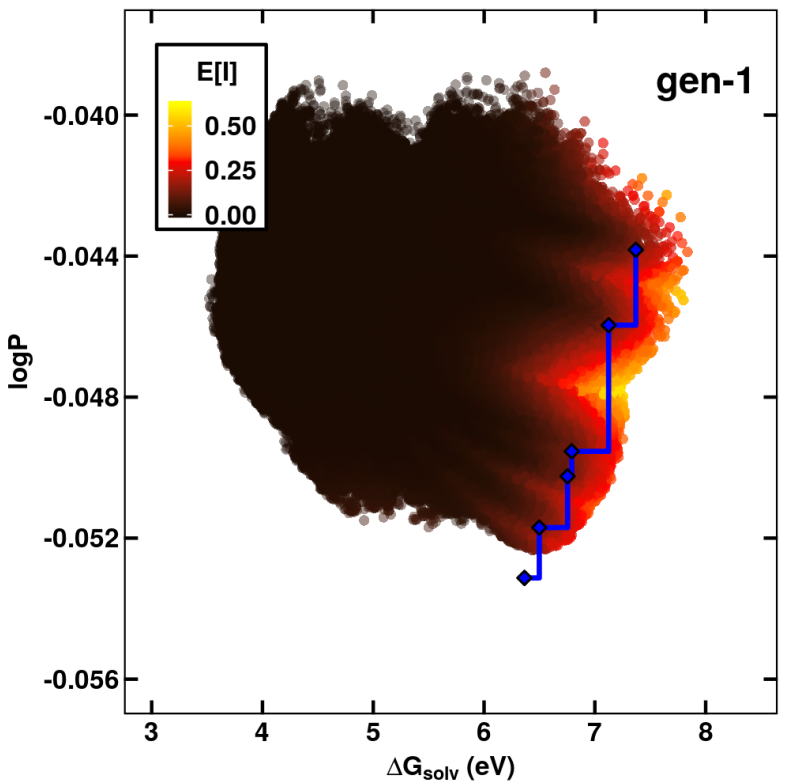

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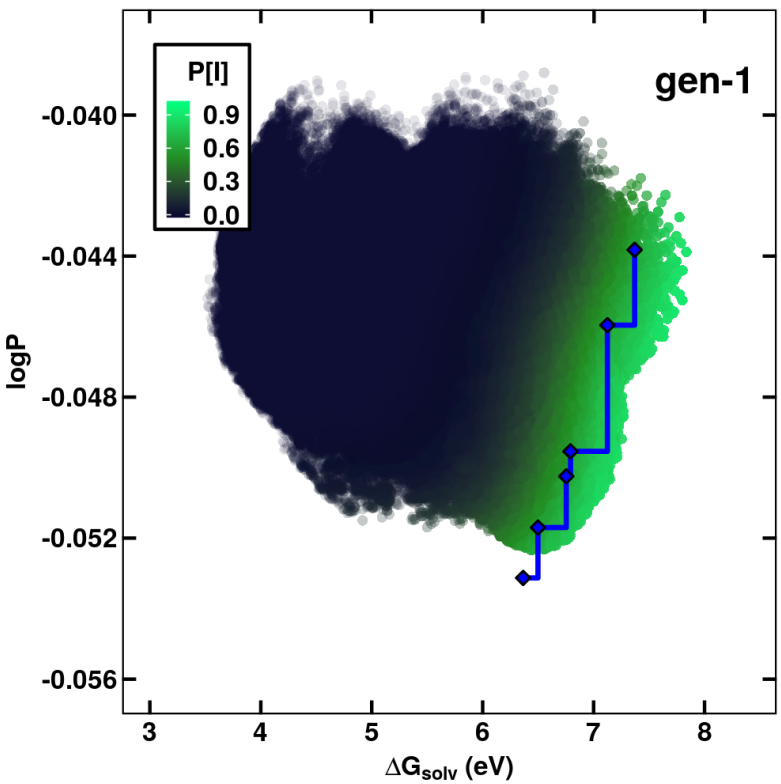

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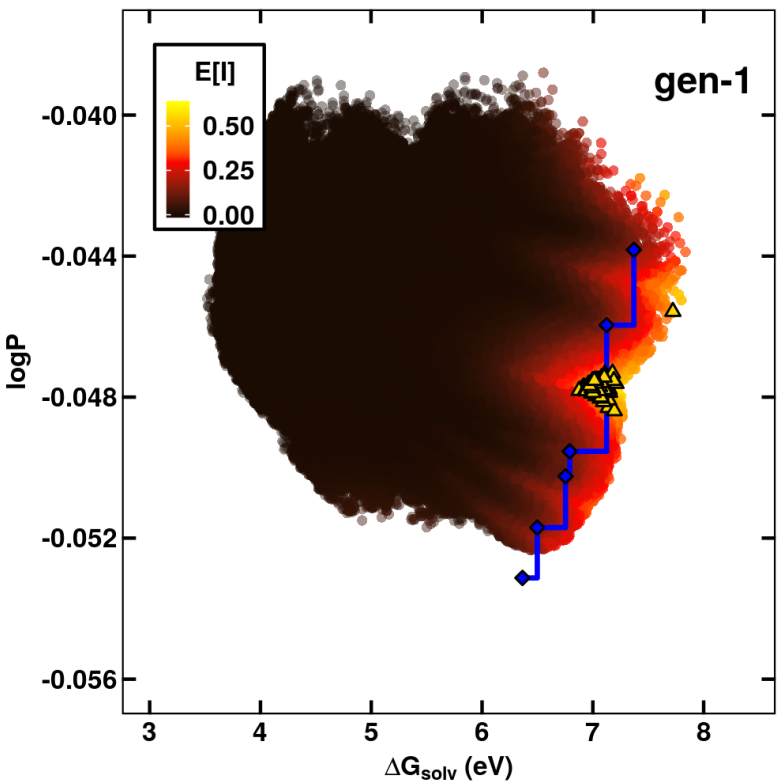

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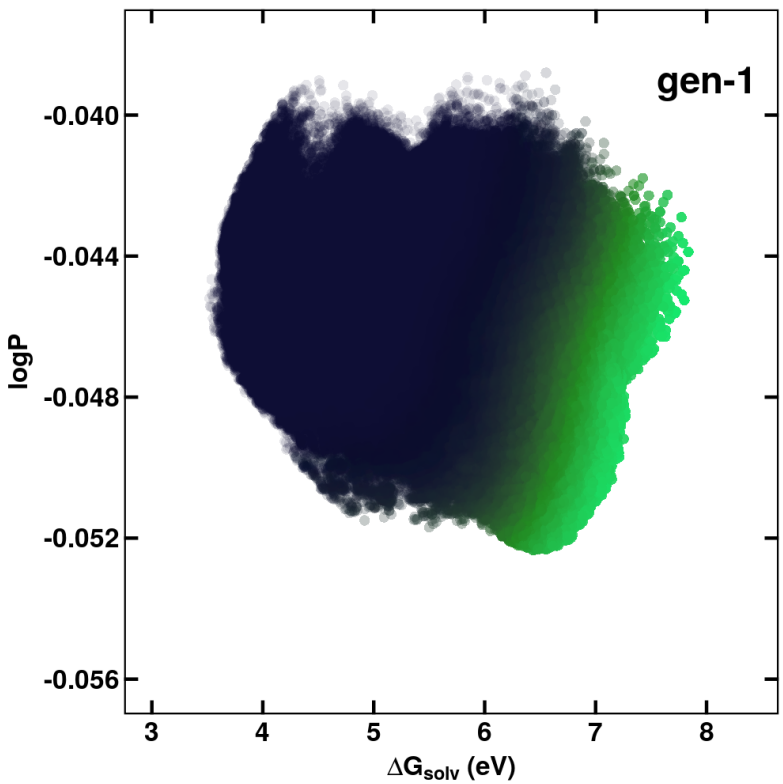
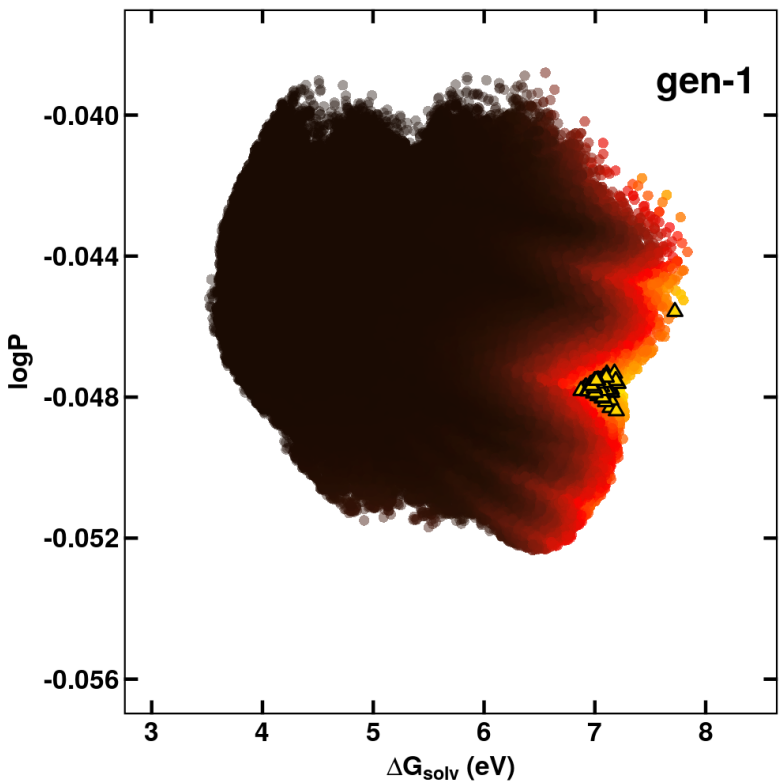
Evolution of PI and EI

probability of improvement



expected improvement



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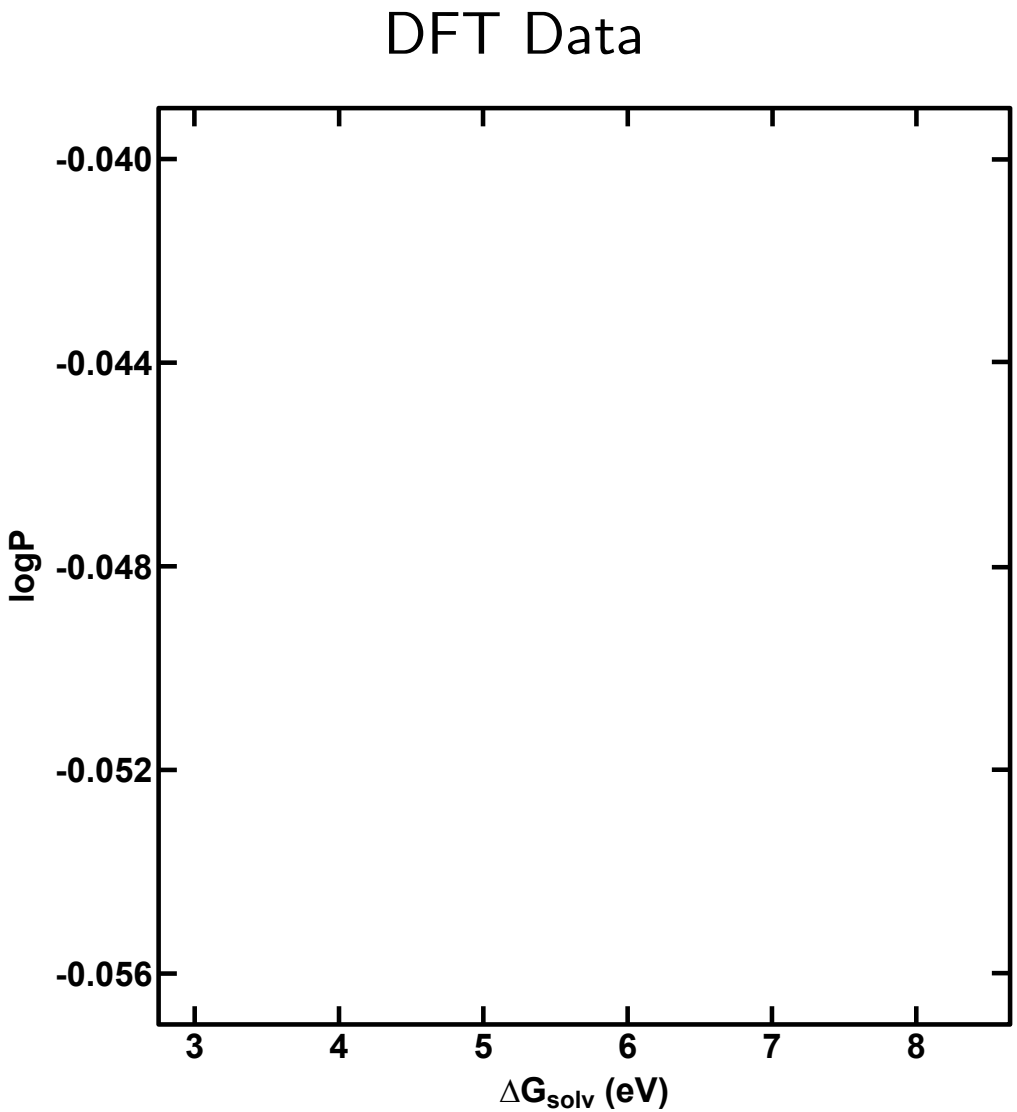
Simulation results



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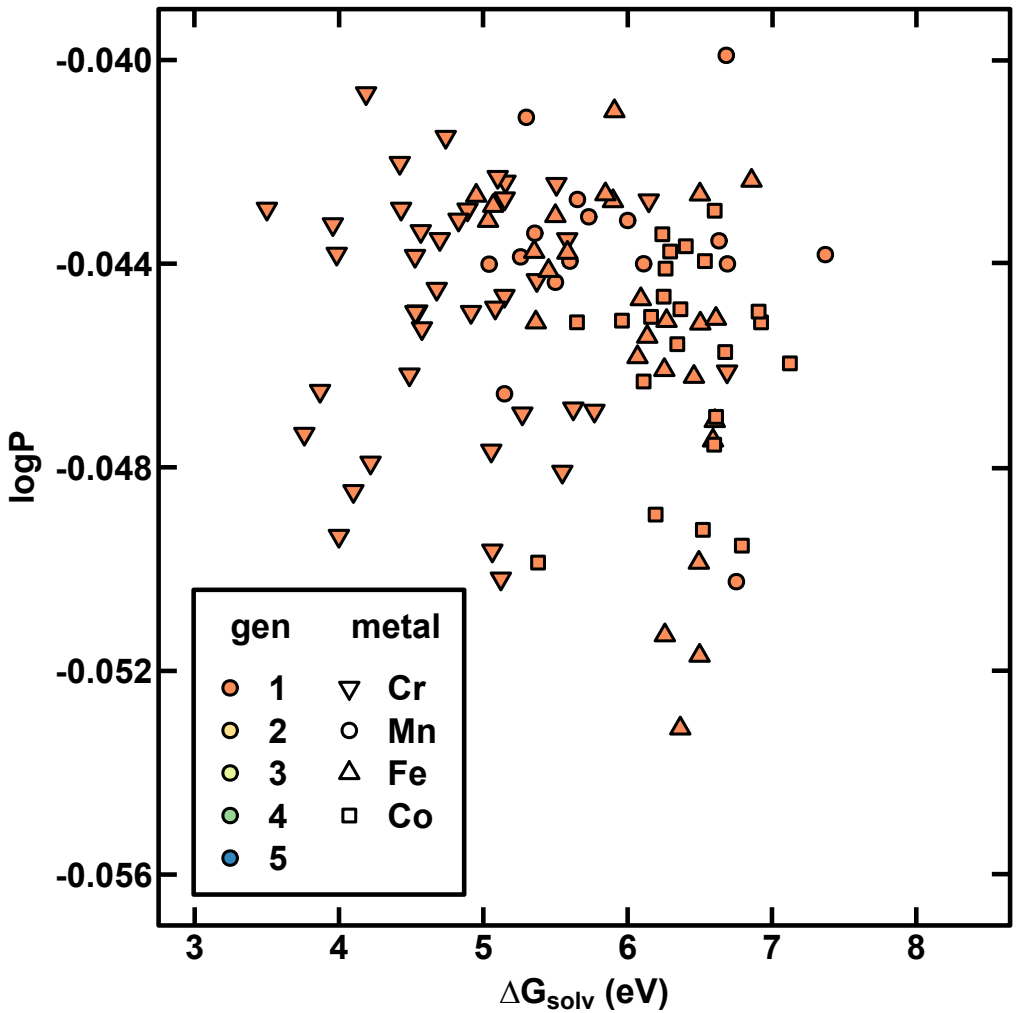
Simulation results

k-medoids points (generation 1)



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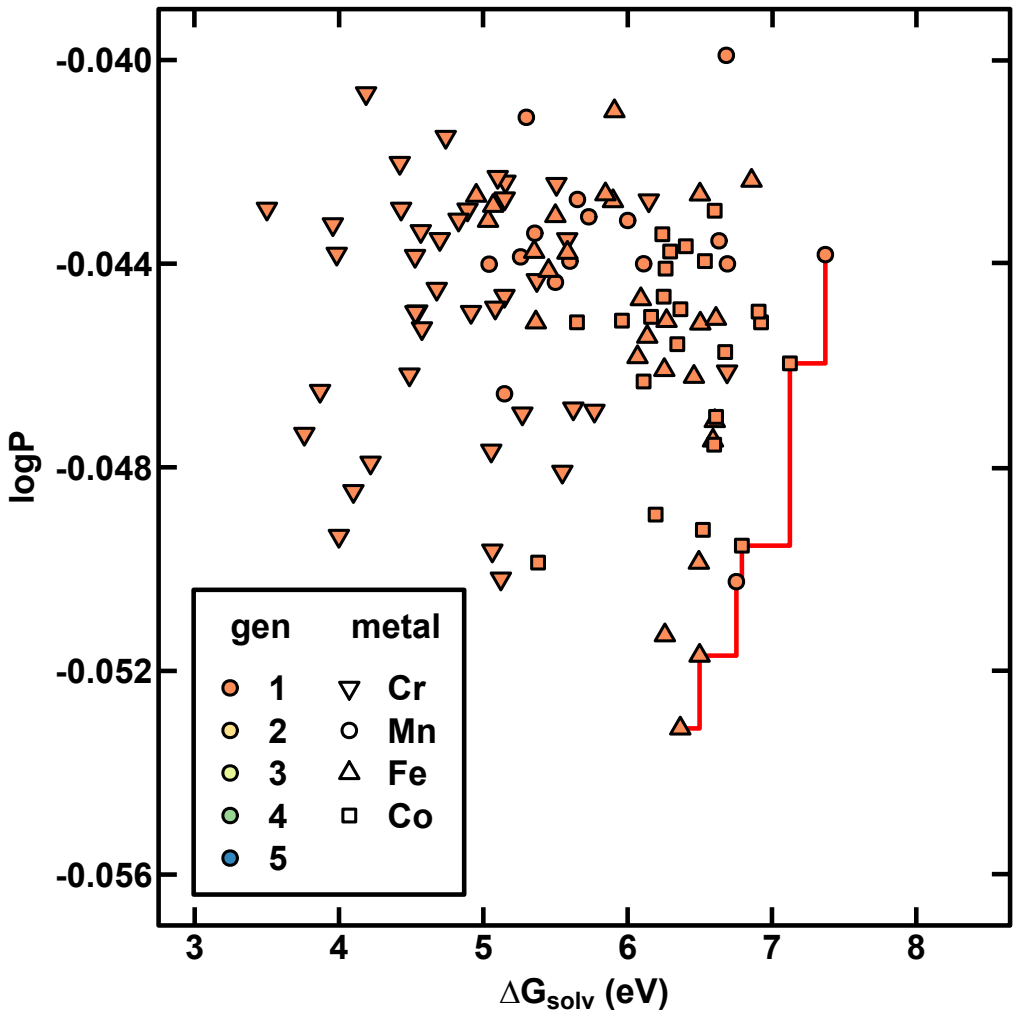
Simulation results

pareto front (generation 1)



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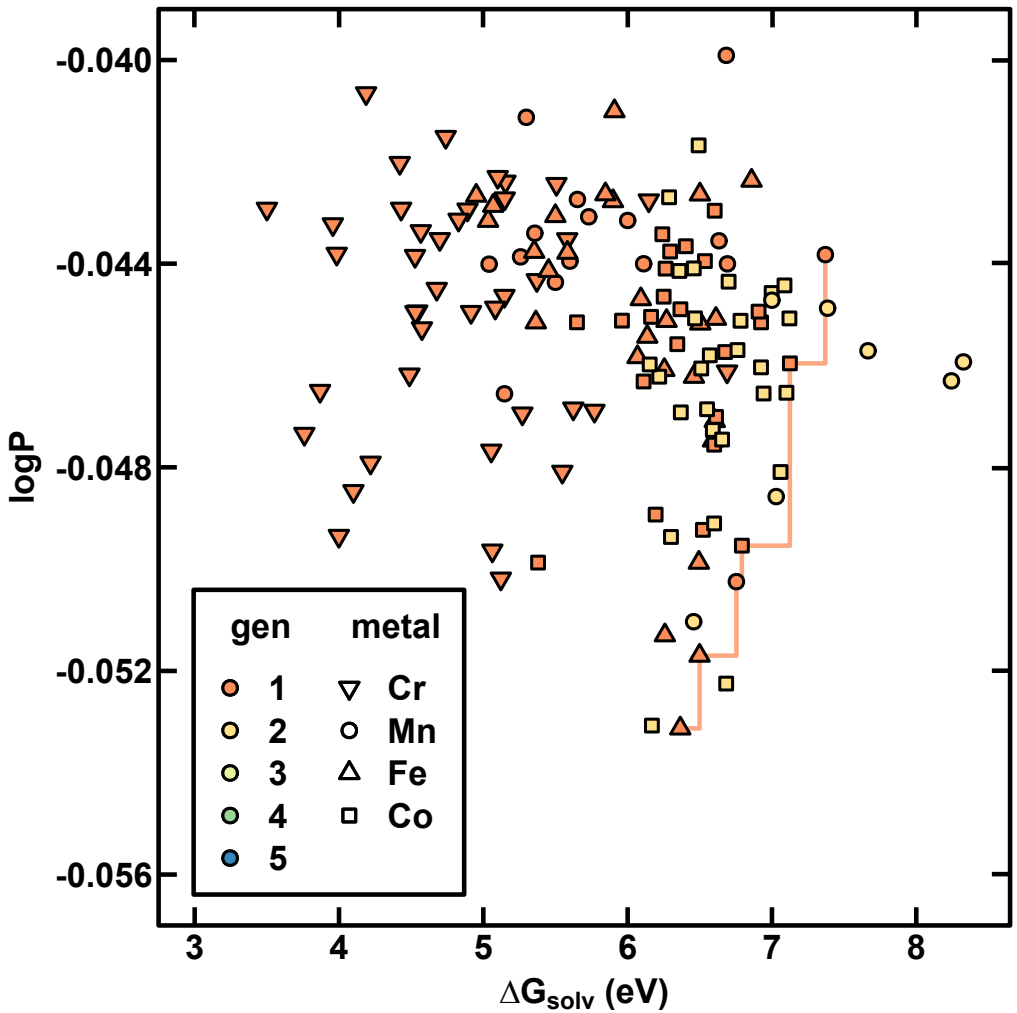
Simulation results

EI points (geneneration 2)



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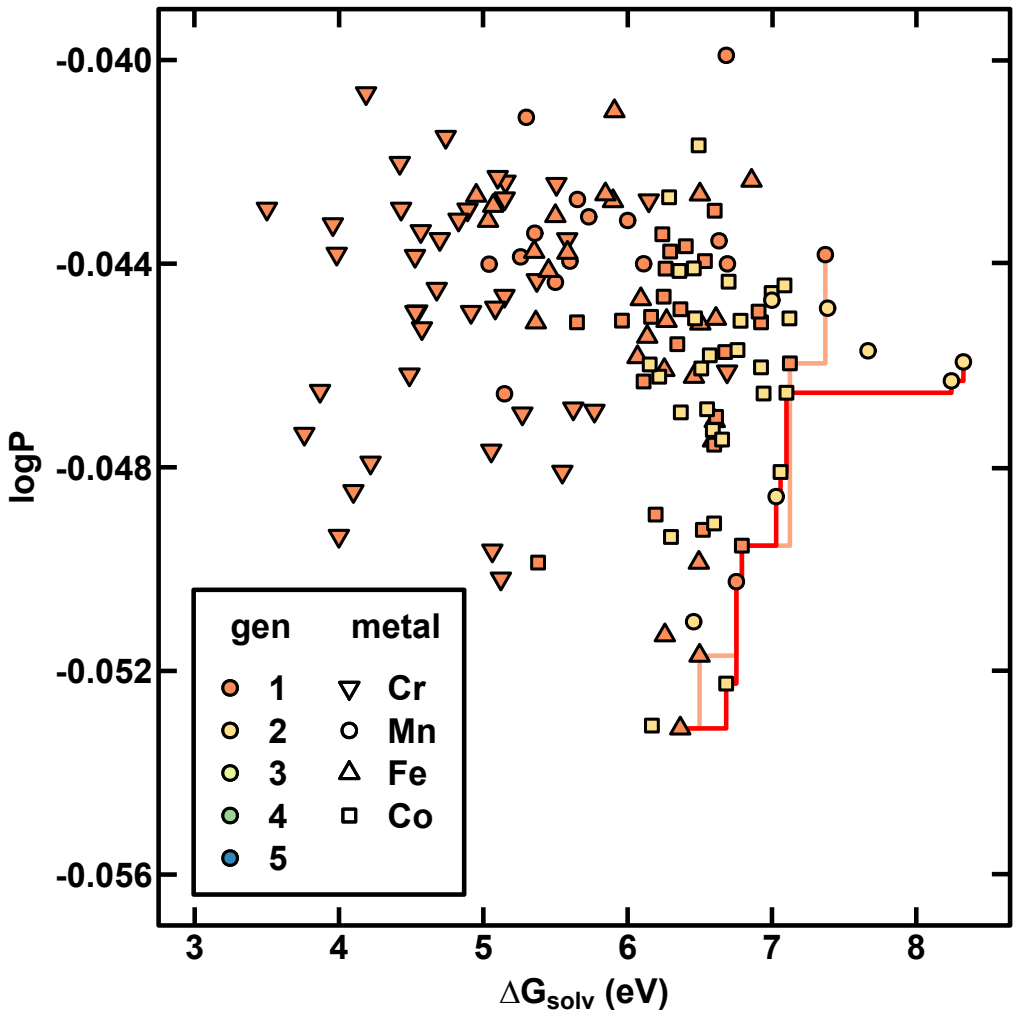

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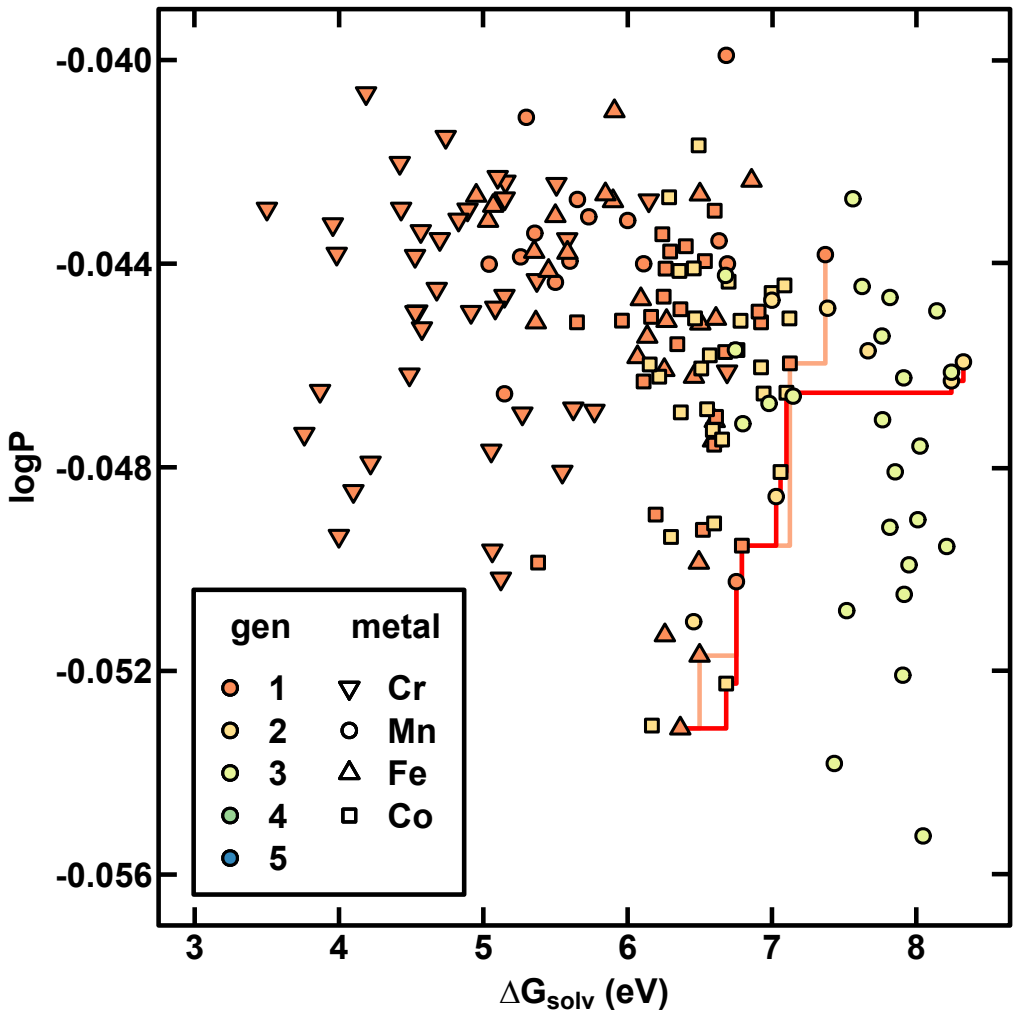

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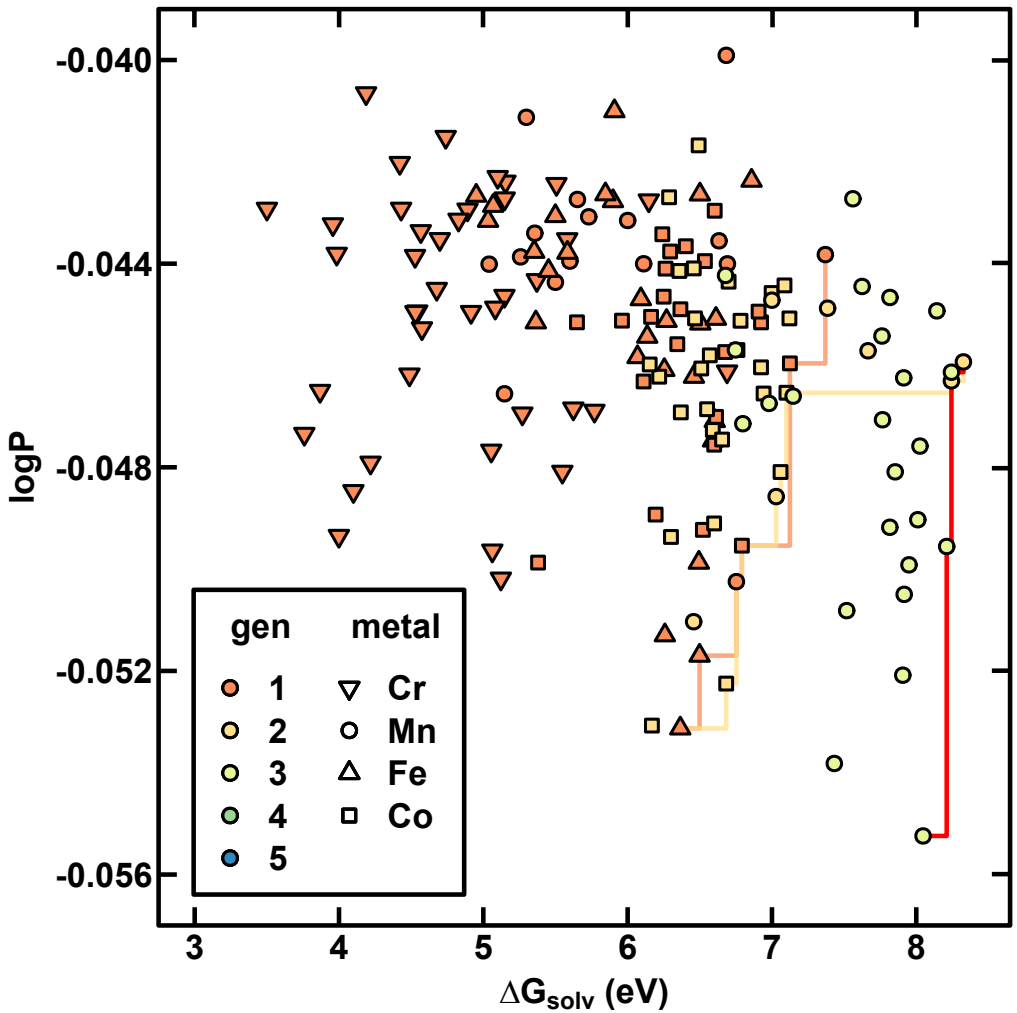

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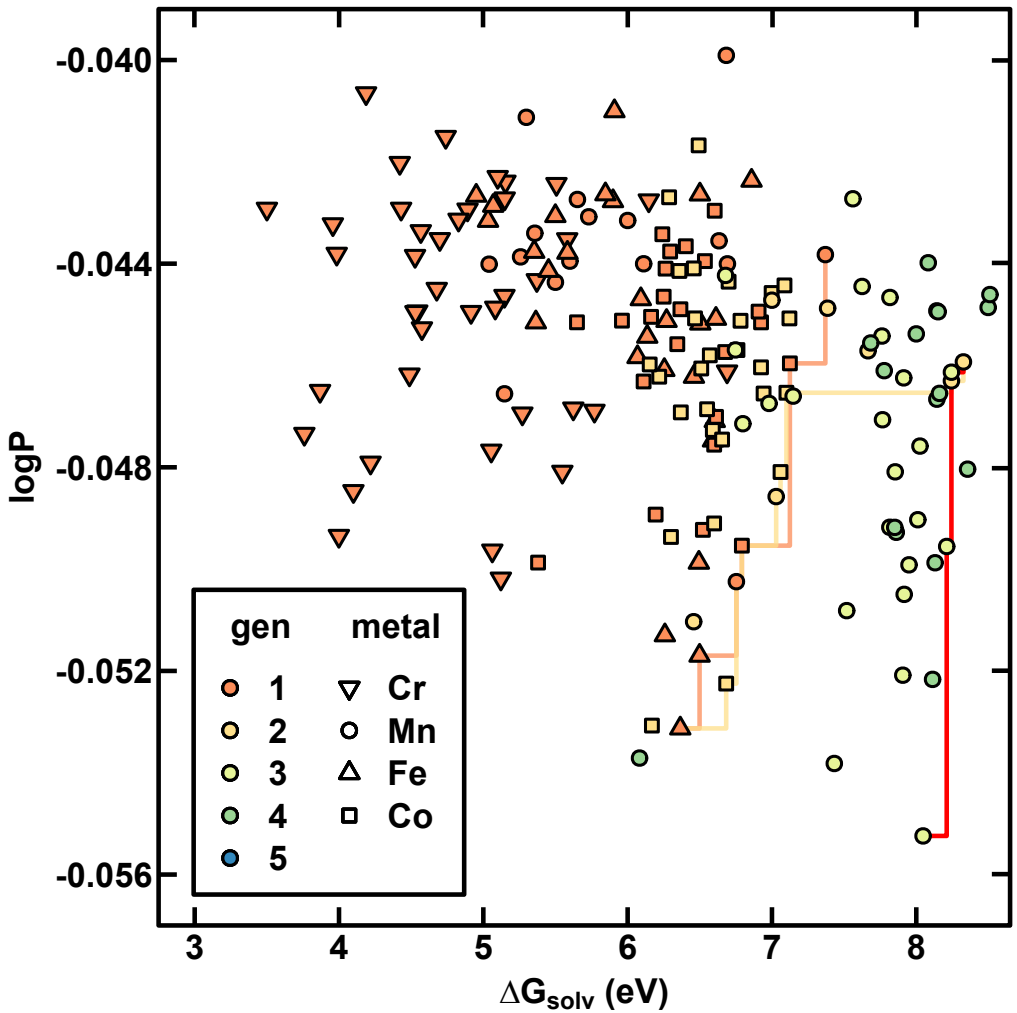
Simulation results

EI points (generation 4)



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Simulation results

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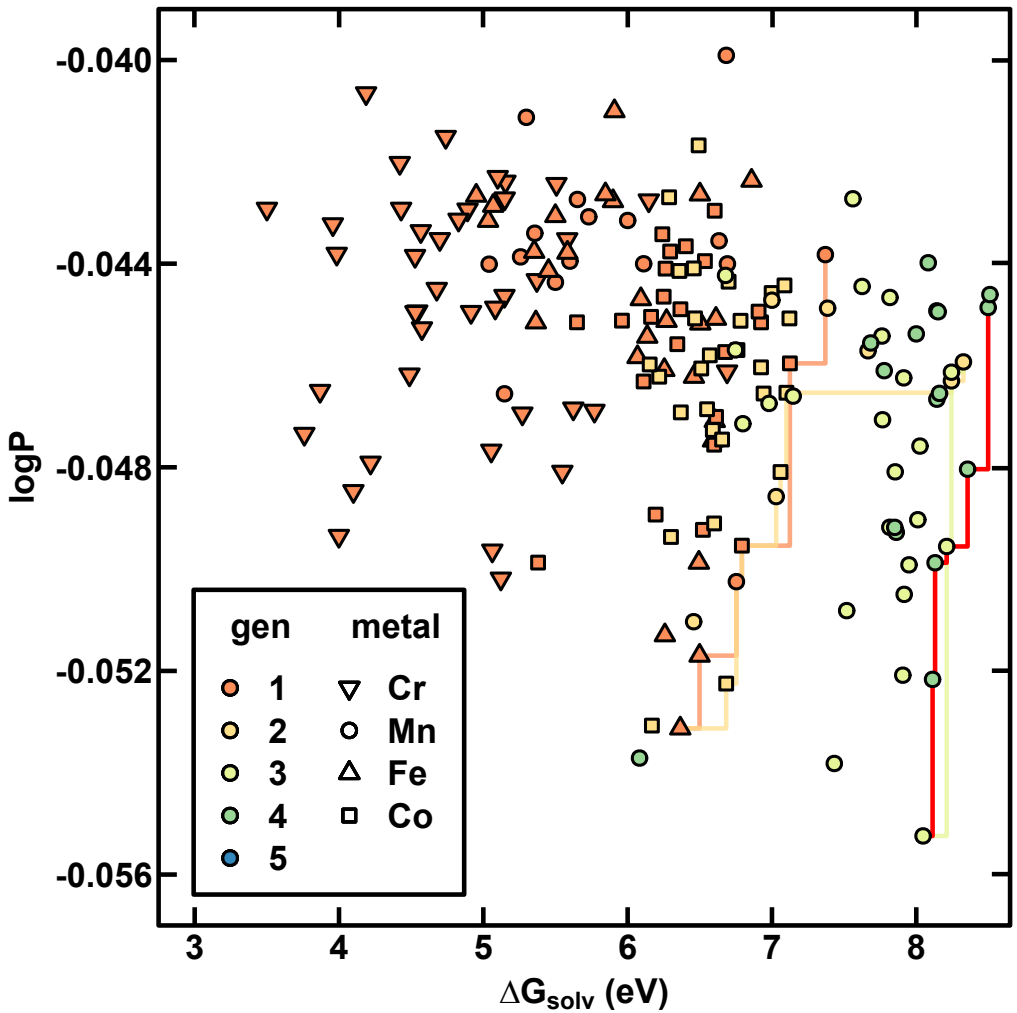

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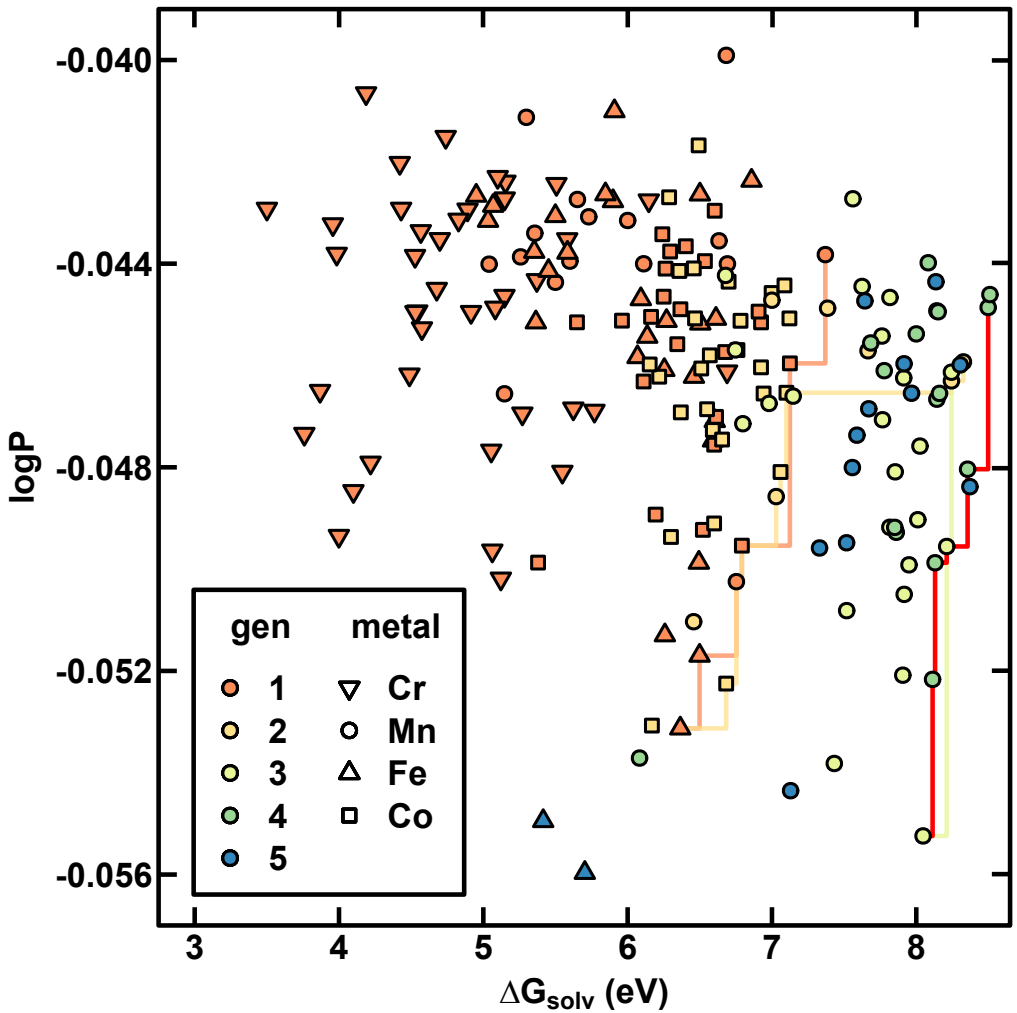
Simulation results

EI points (generation 5)



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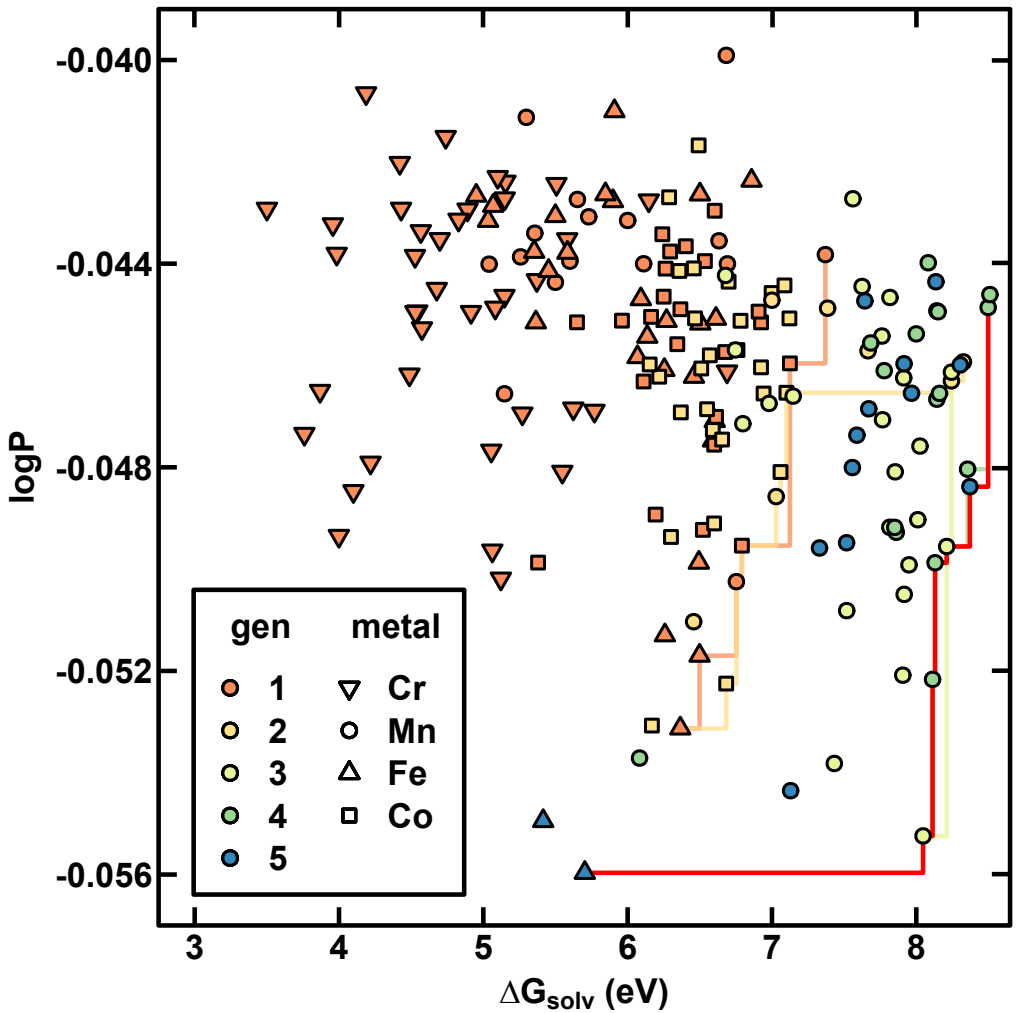

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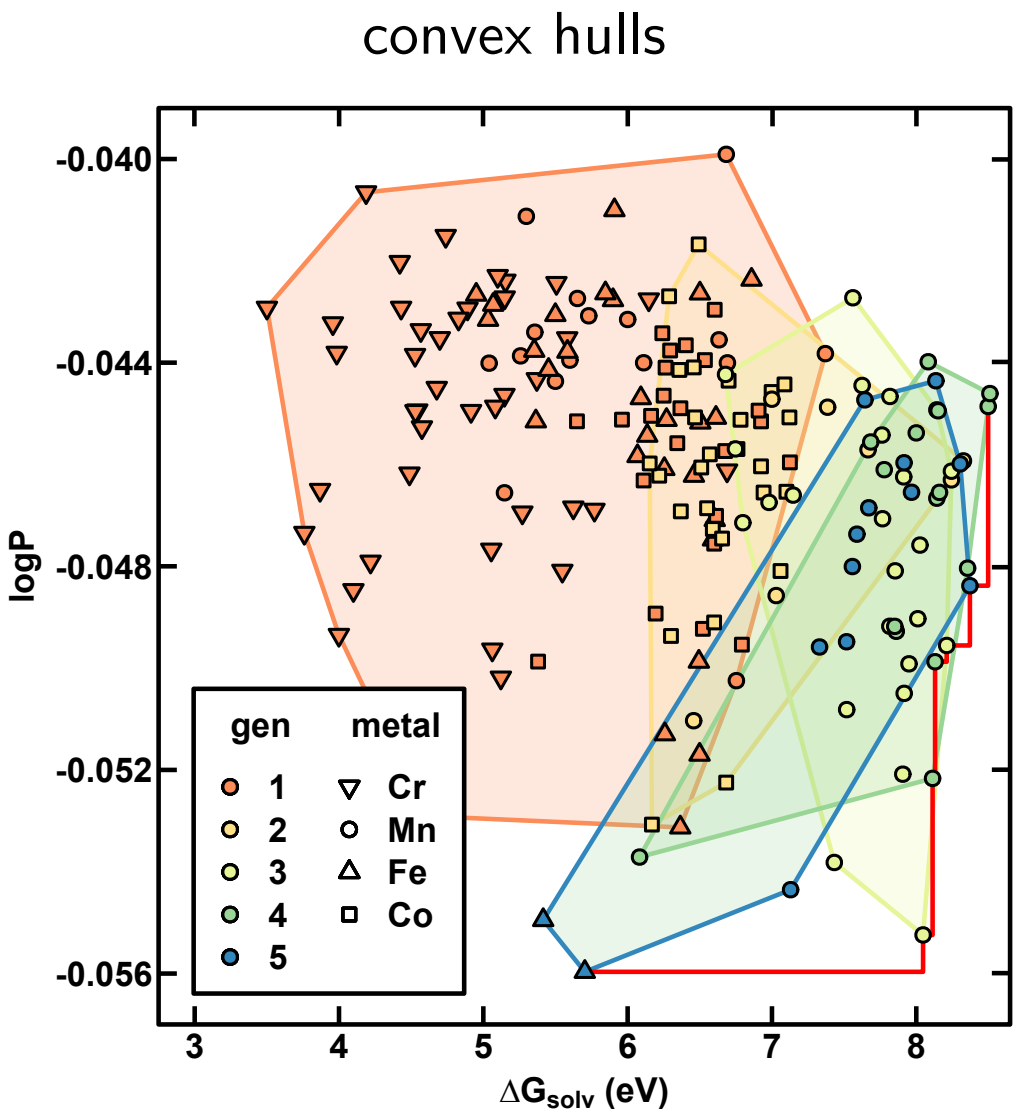

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Conclusions

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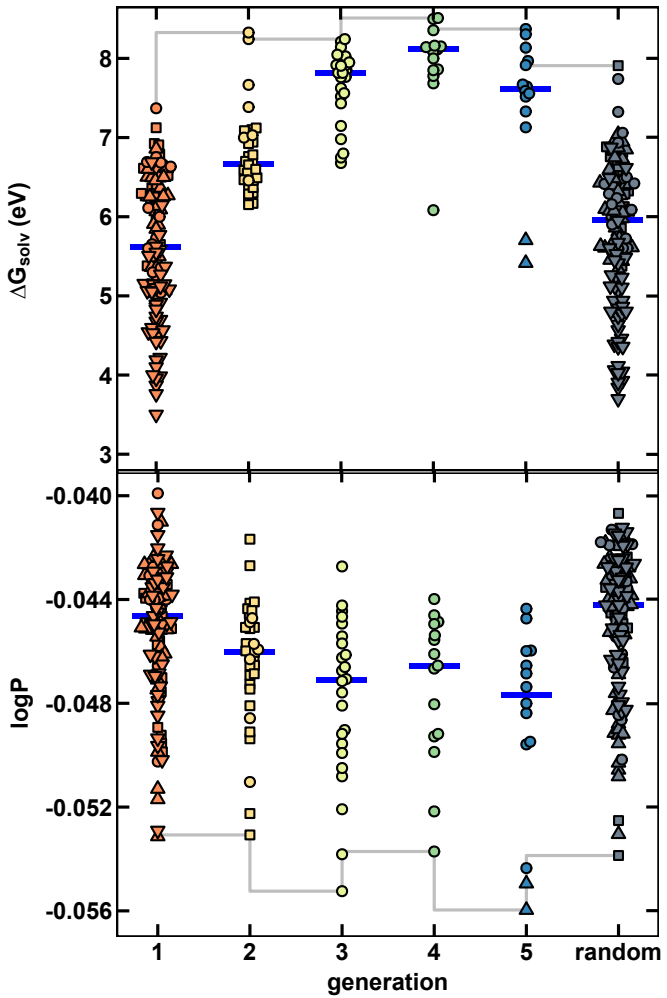
- EI framework provides high resolution in the region of interest (c.f. maximum uncertainty), converges quickly



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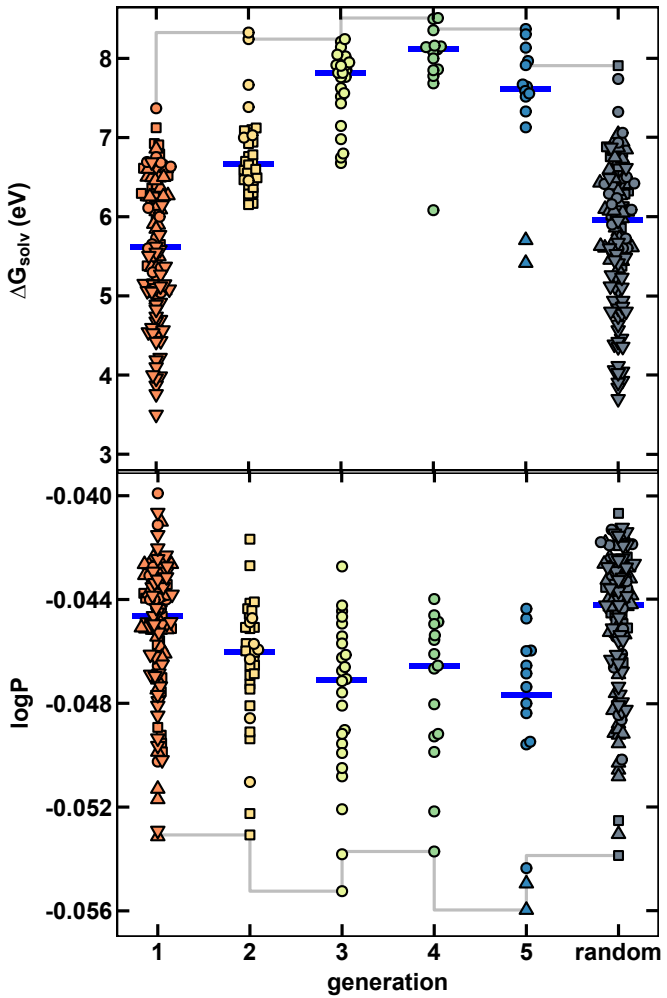
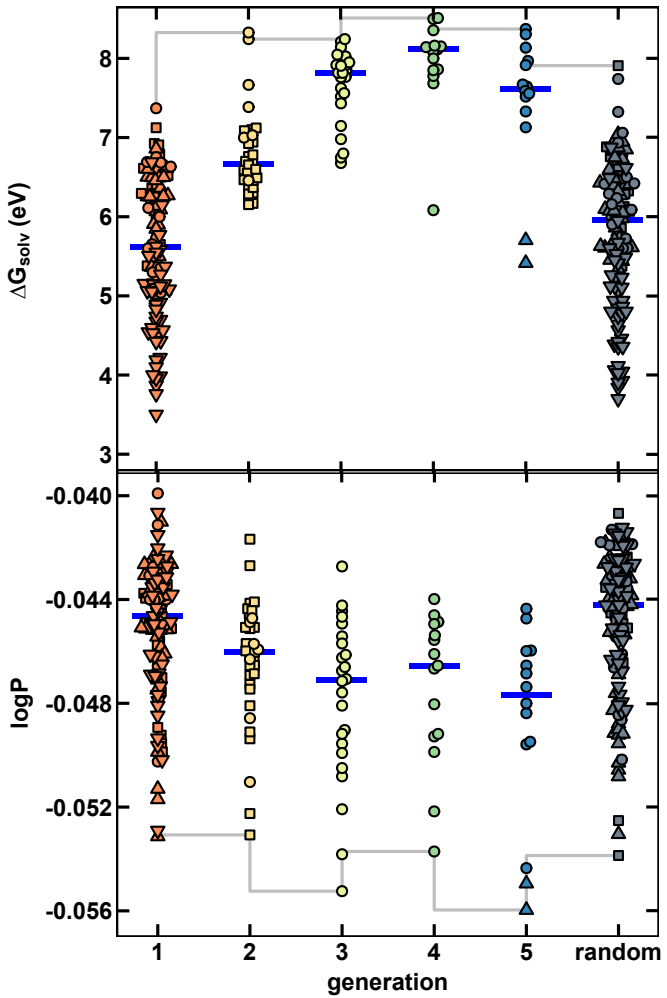


Conclusions

- EI framework provides high resolution in the region of interest (c.f. maximum uncertainty), converges quickly
- We are able to identify fruitful regions from large chemical spaces based on few DFT evaluations
- Multiobjective DFT optimization guided by data-driven method efficiency generates lead complexes



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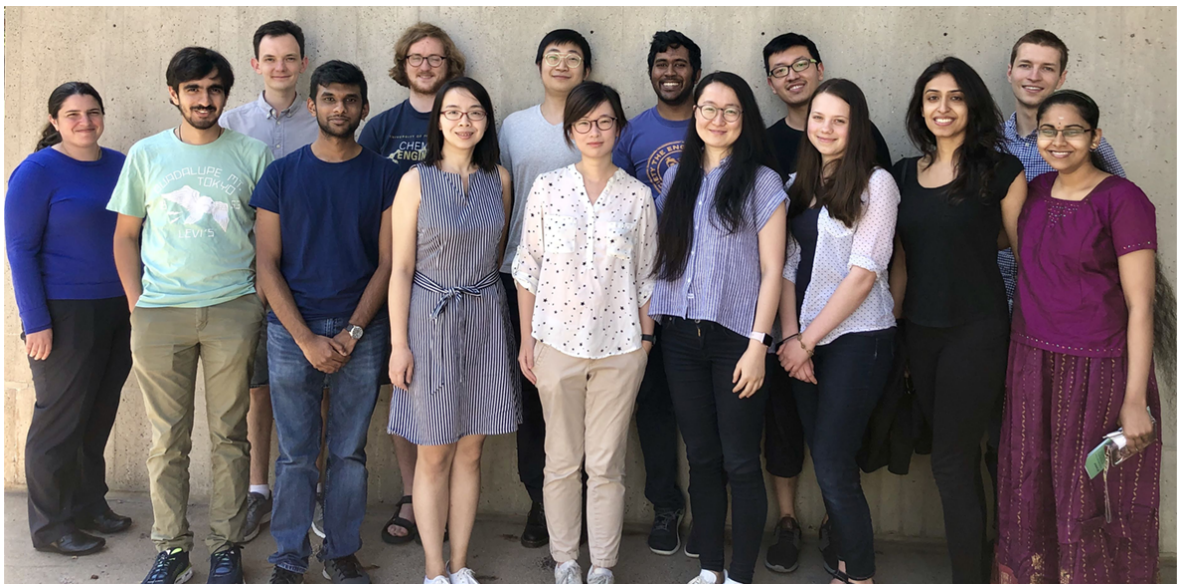
Acknowledgments

This work is thanks to the Kulik group and funding partners:



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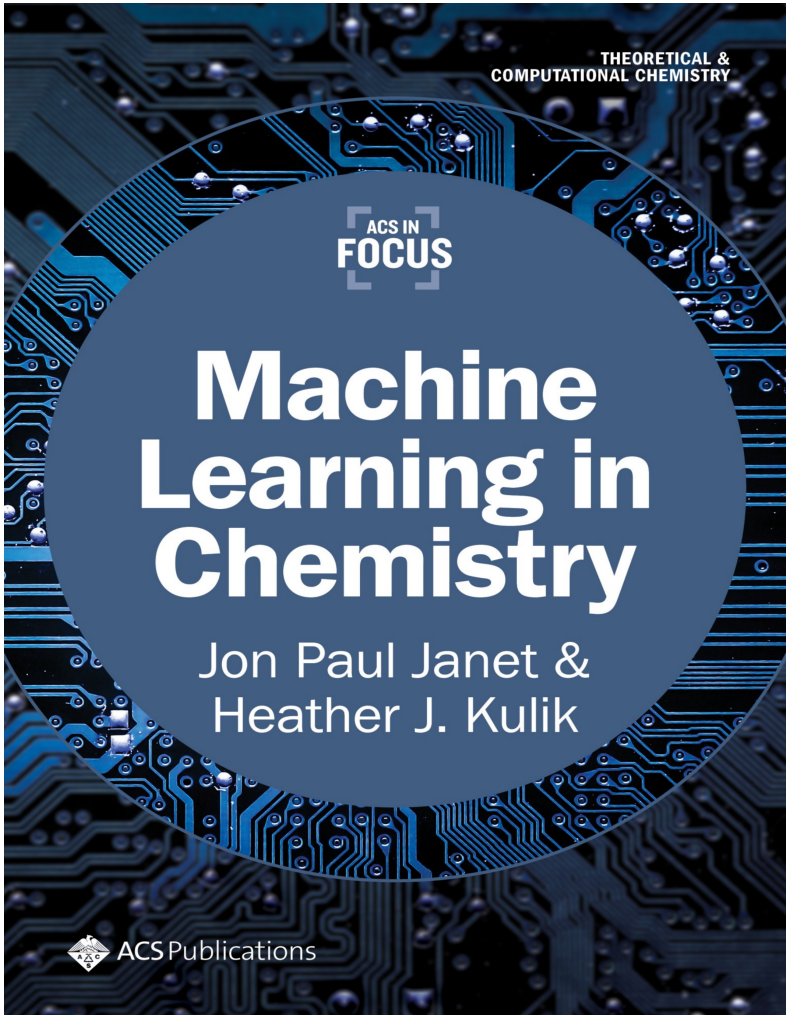

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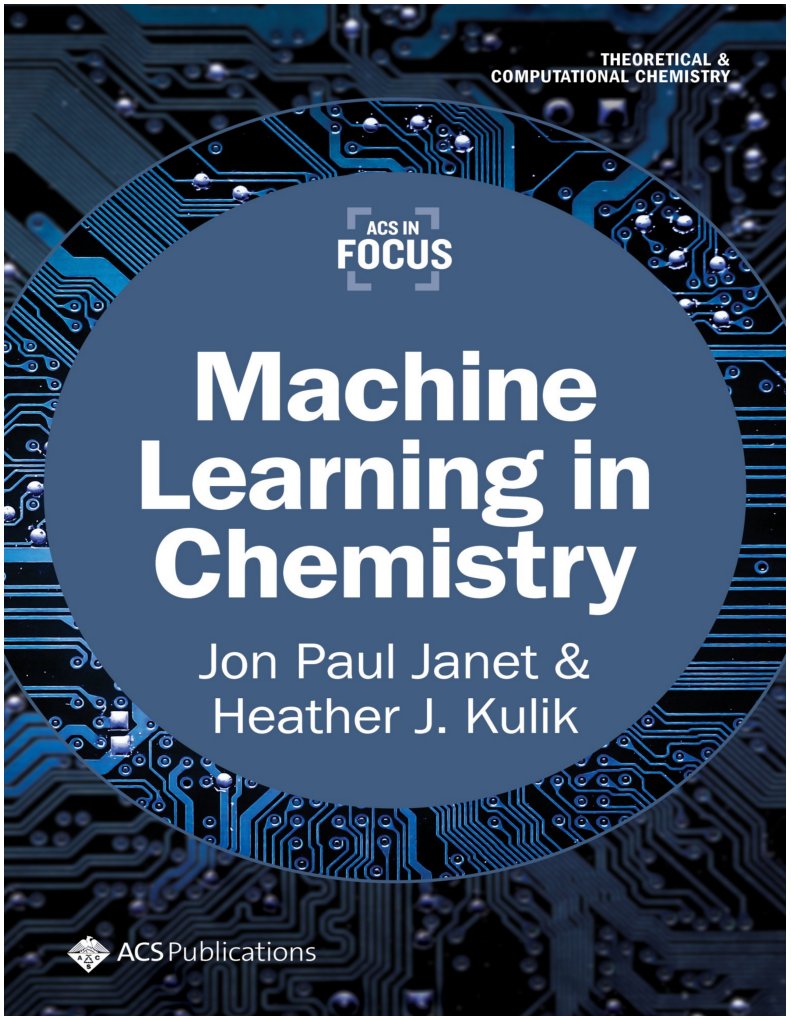

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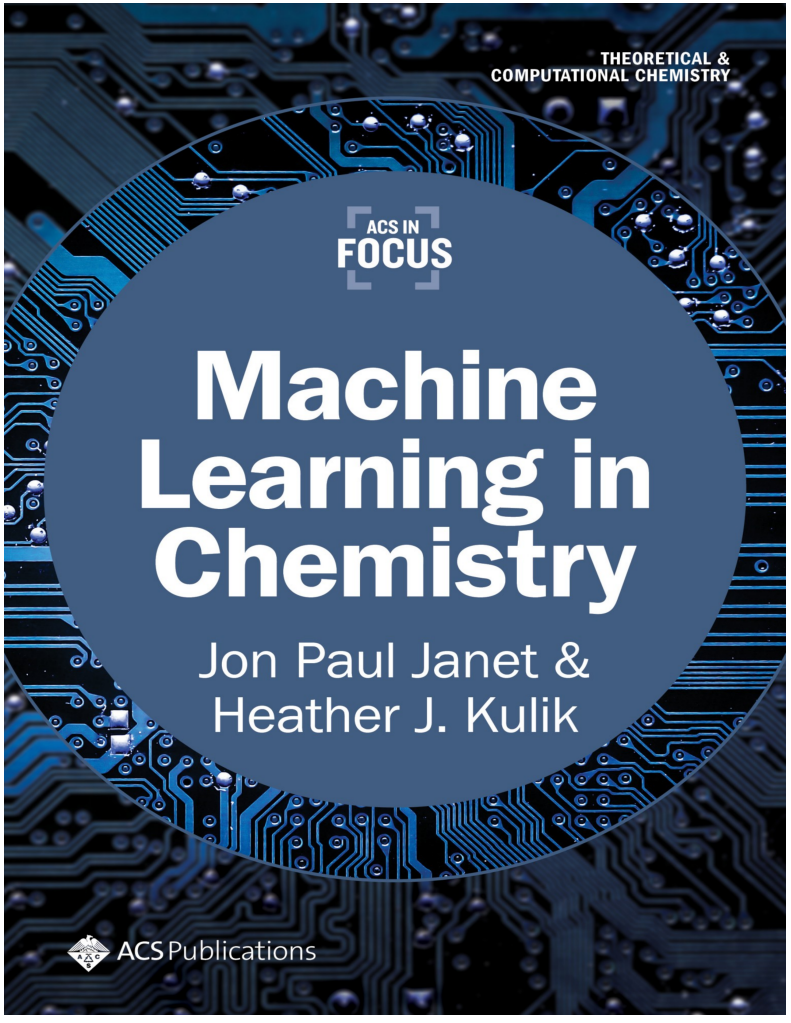

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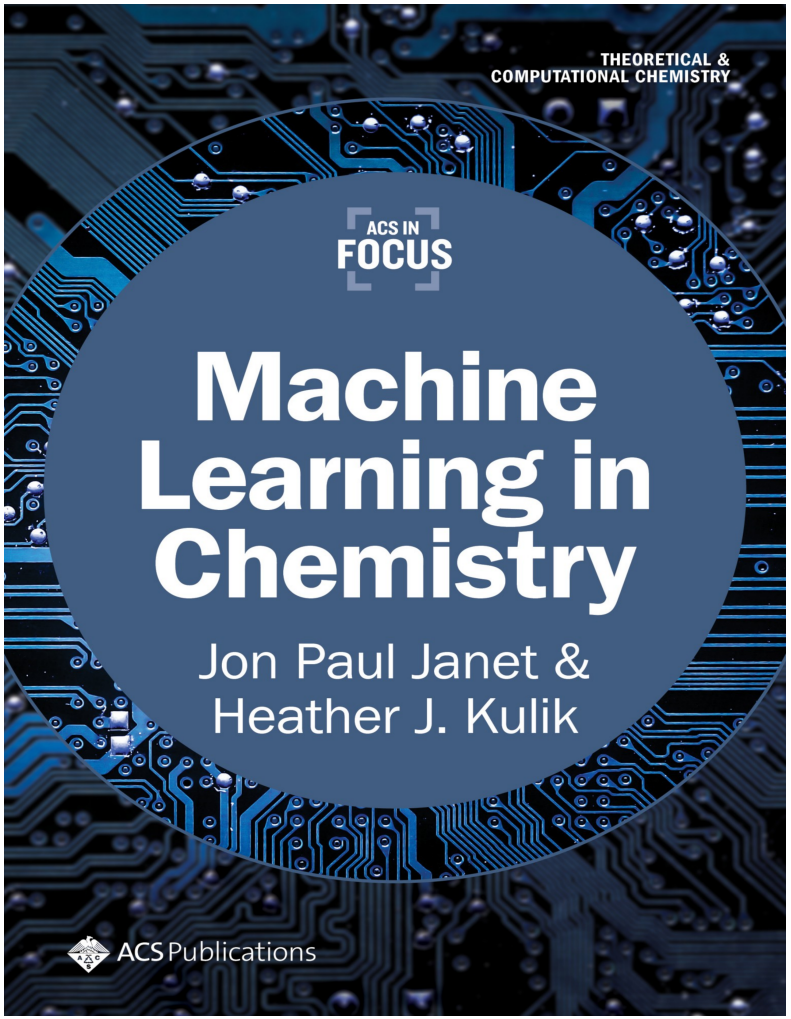

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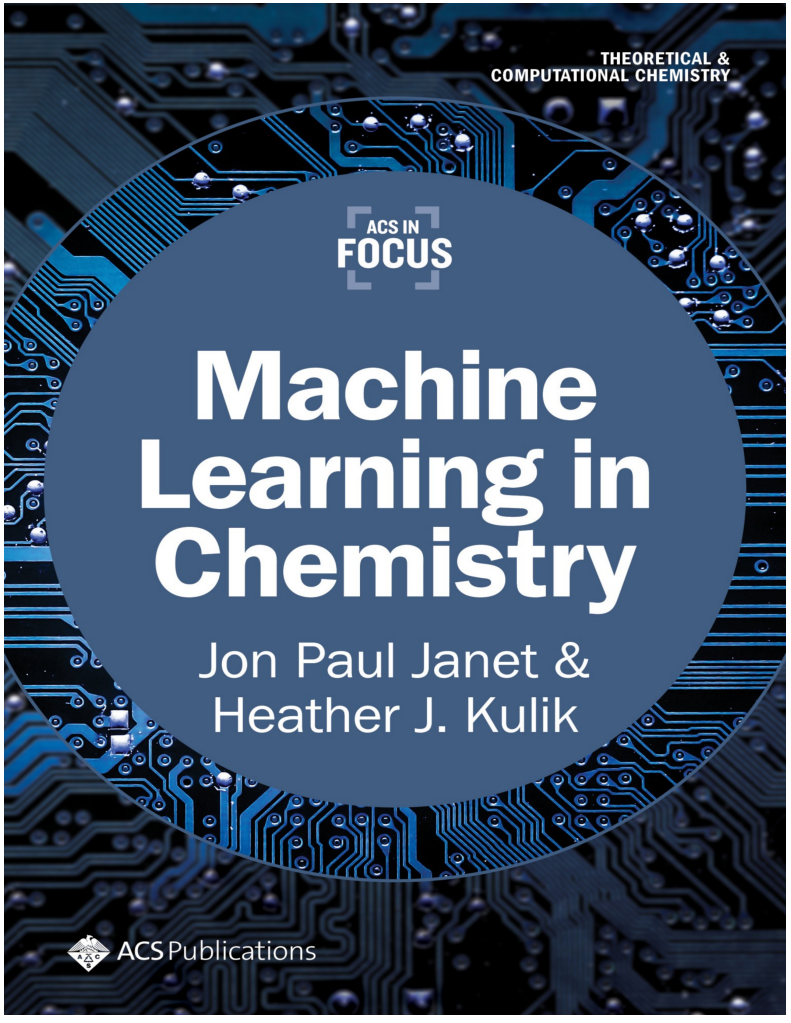

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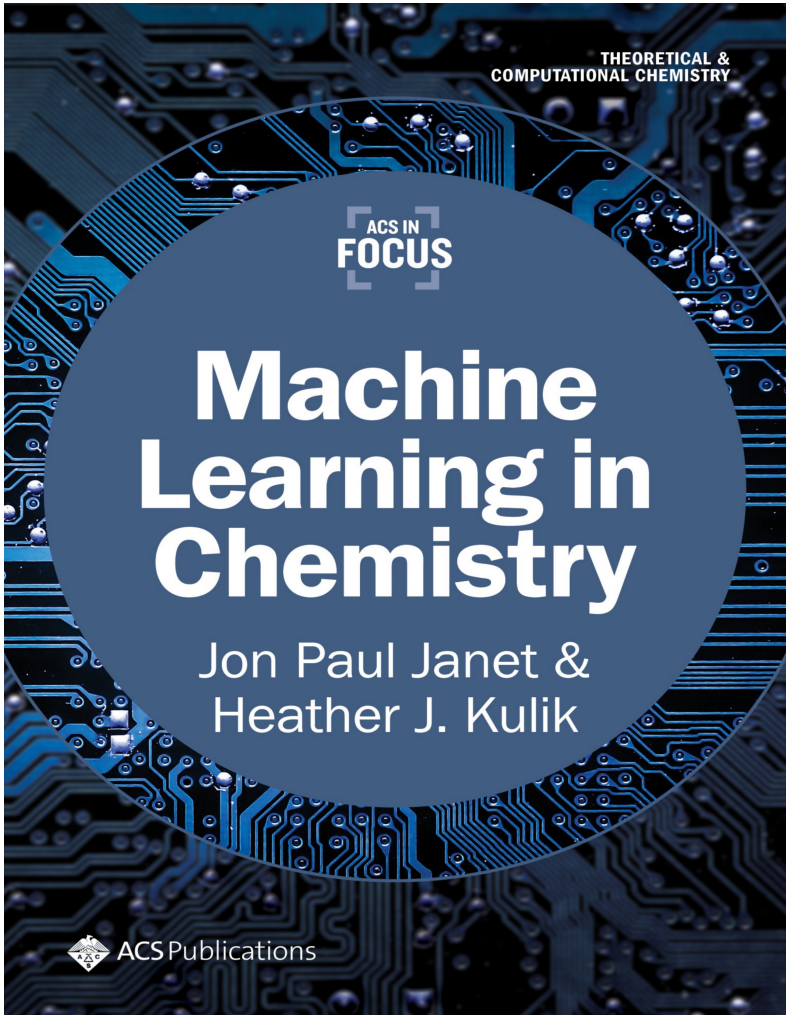

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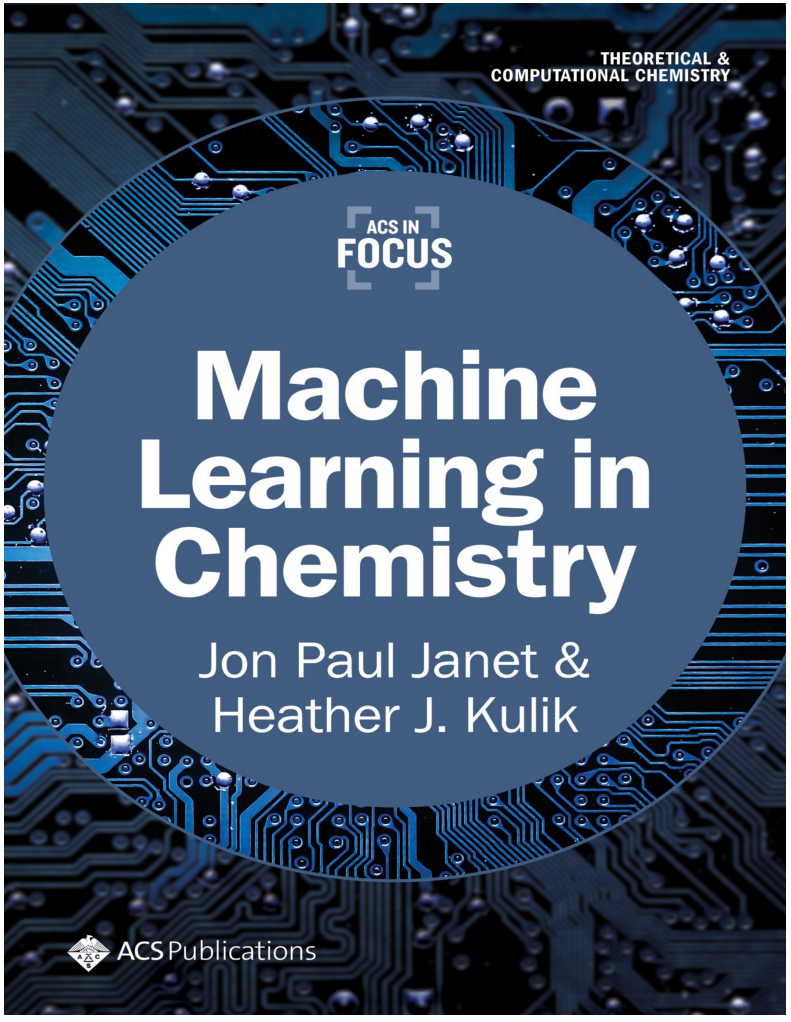

C2: Supervised learning

Supervised learning methods attempt to connect patterns in data to known endpoints by learning model parameters that reproduce the observed relationship.

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observation property

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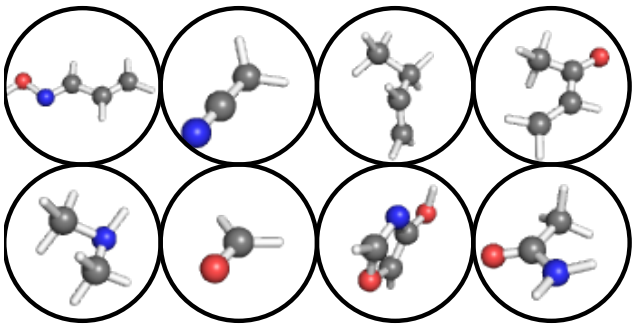

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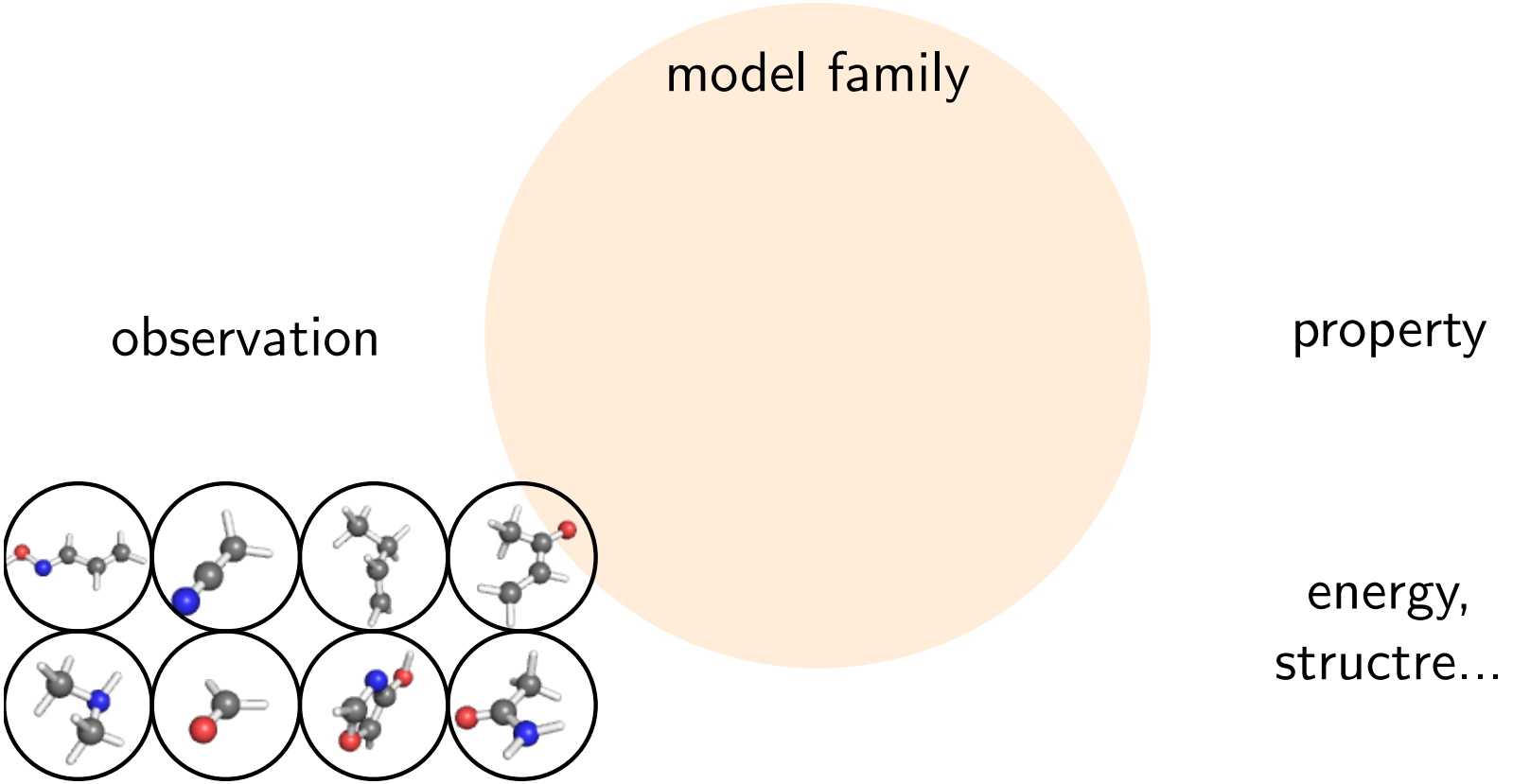

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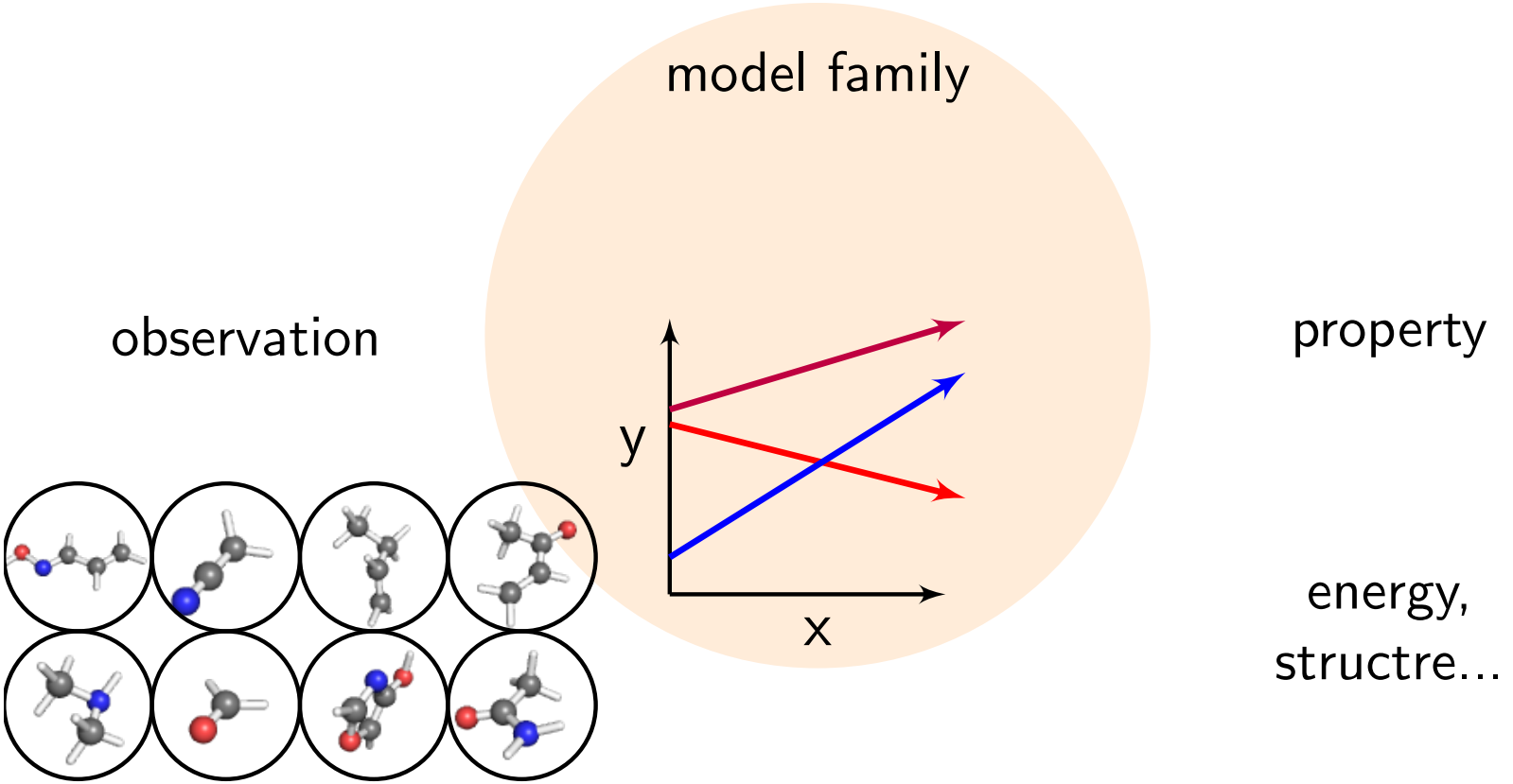

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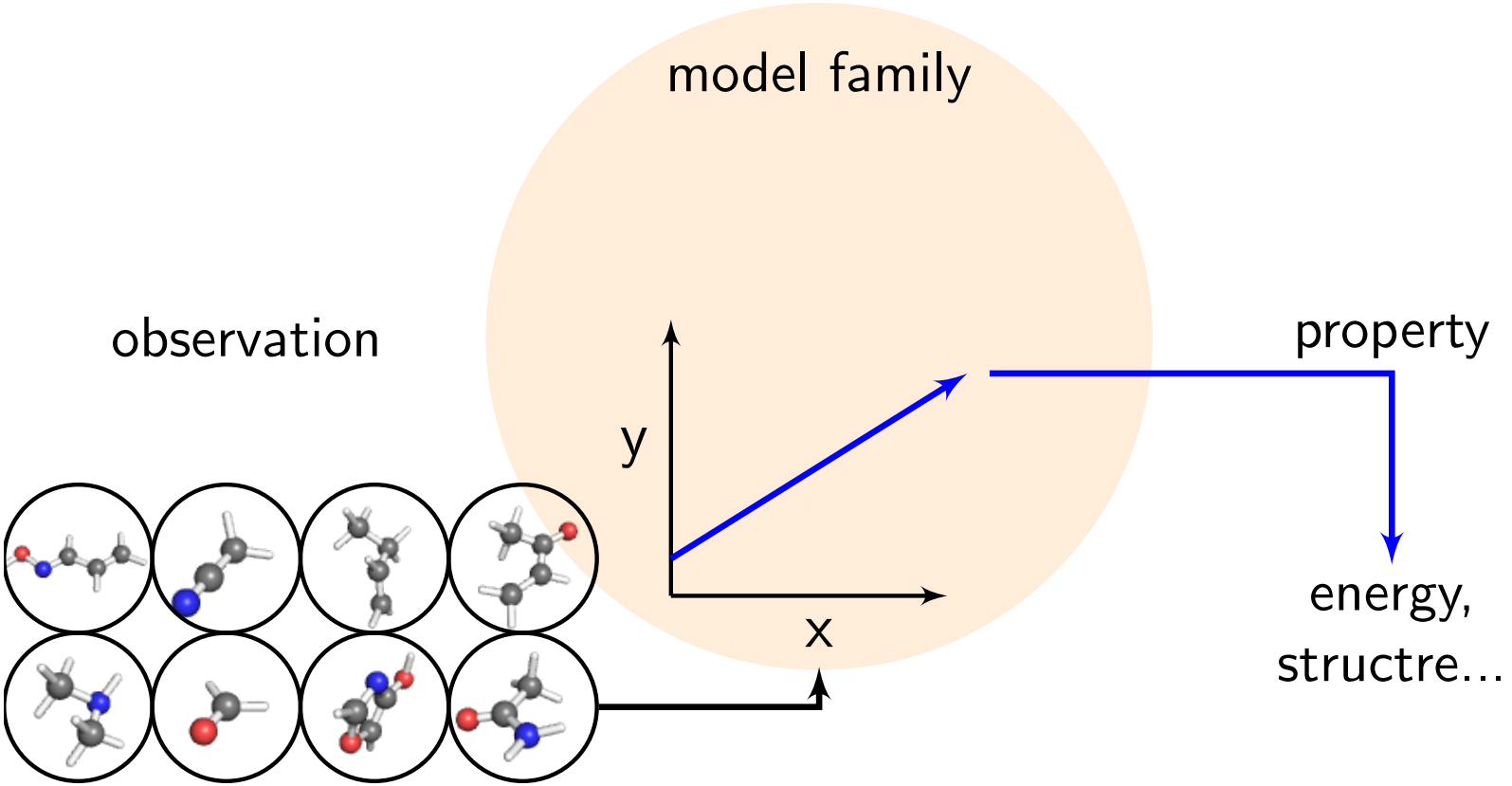

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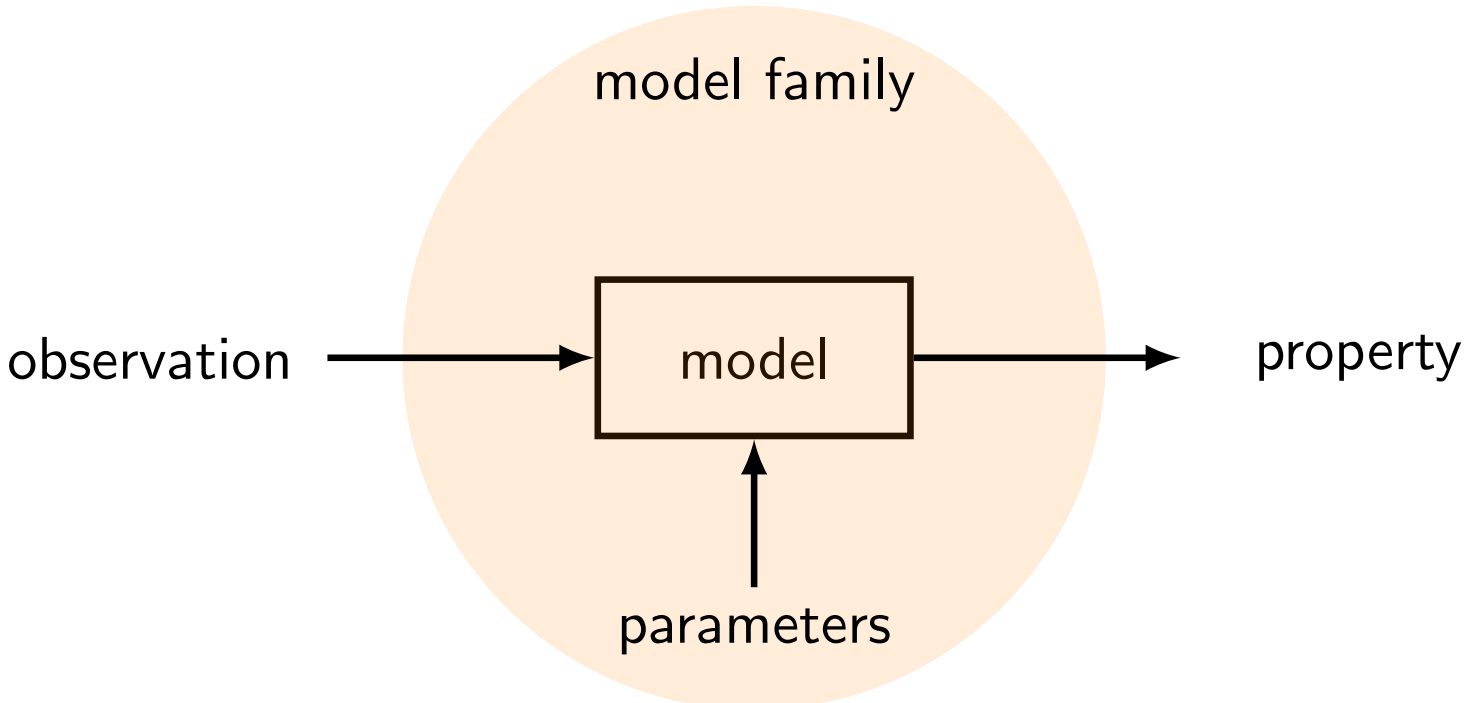

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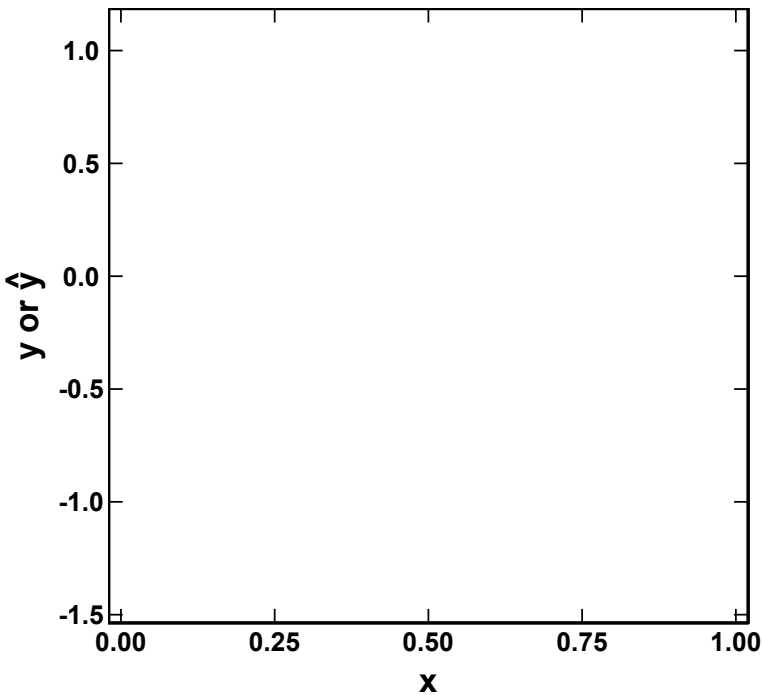

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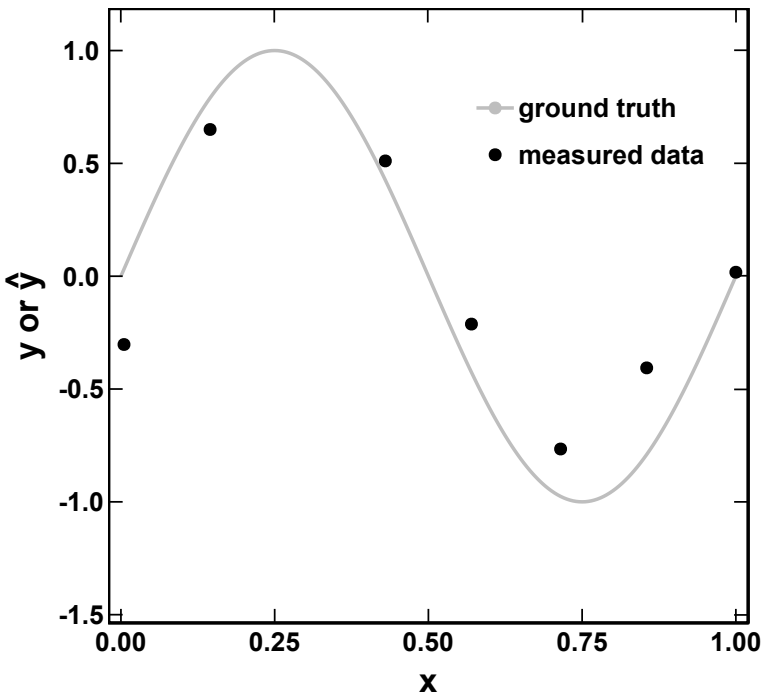
Assume 8 measurements with noise $\mathcal{N}(0, 0.2)$



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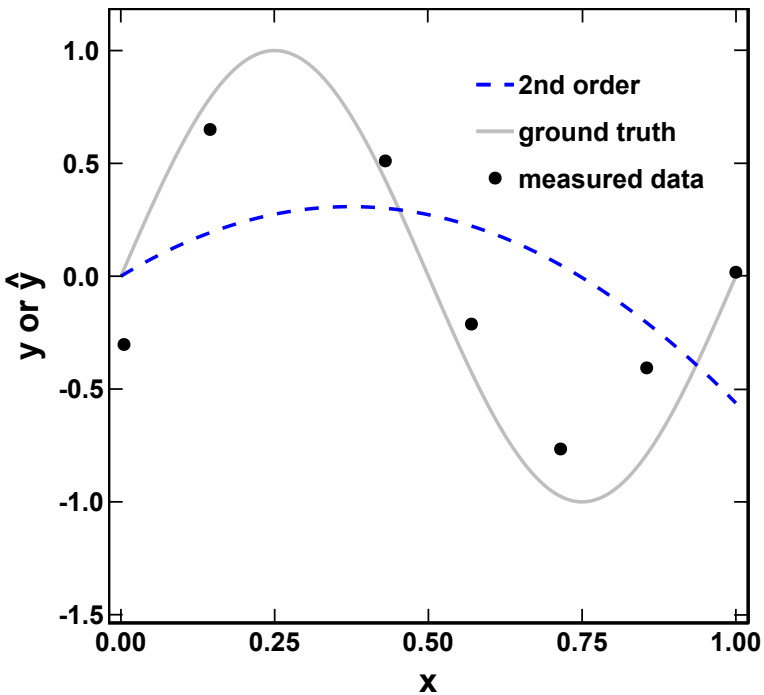

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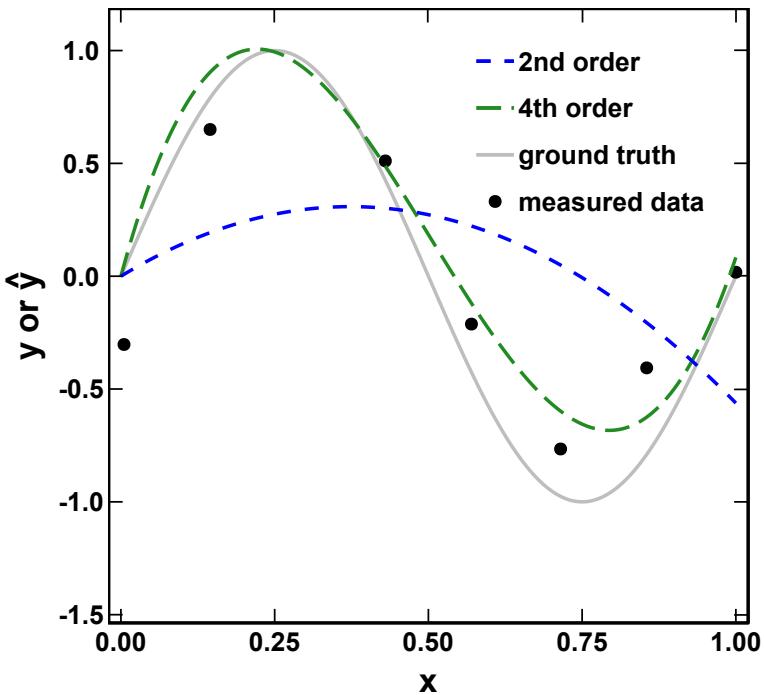

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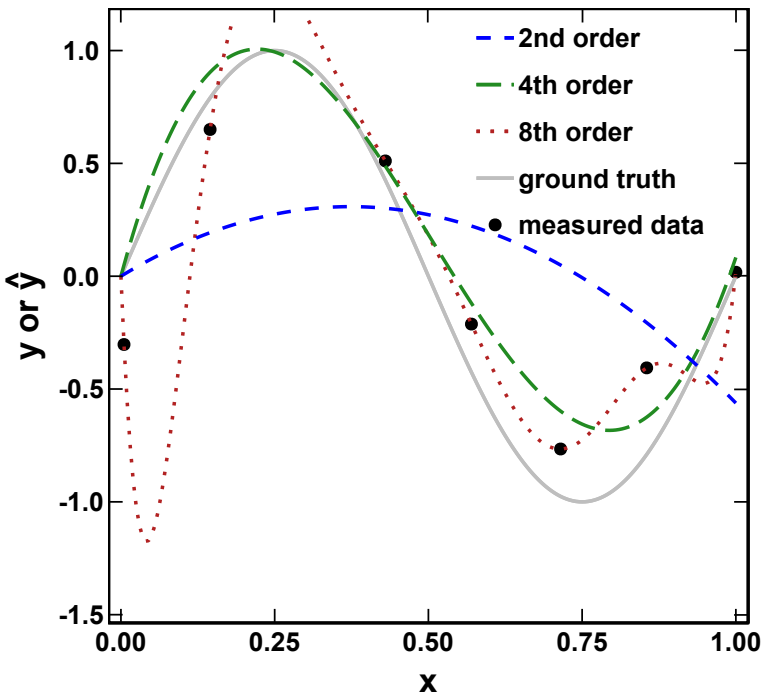

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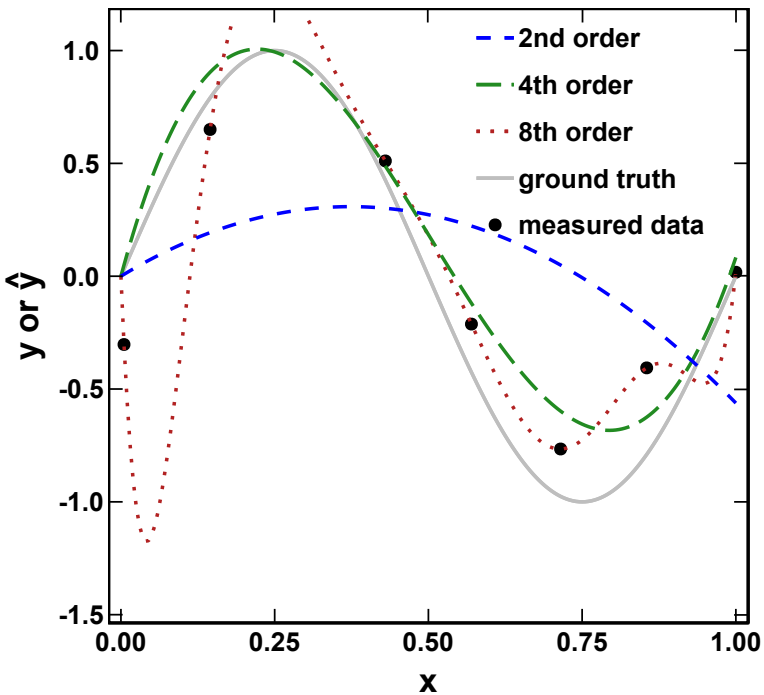
Empirical risk: error on training data

True risk: error over the whole domain



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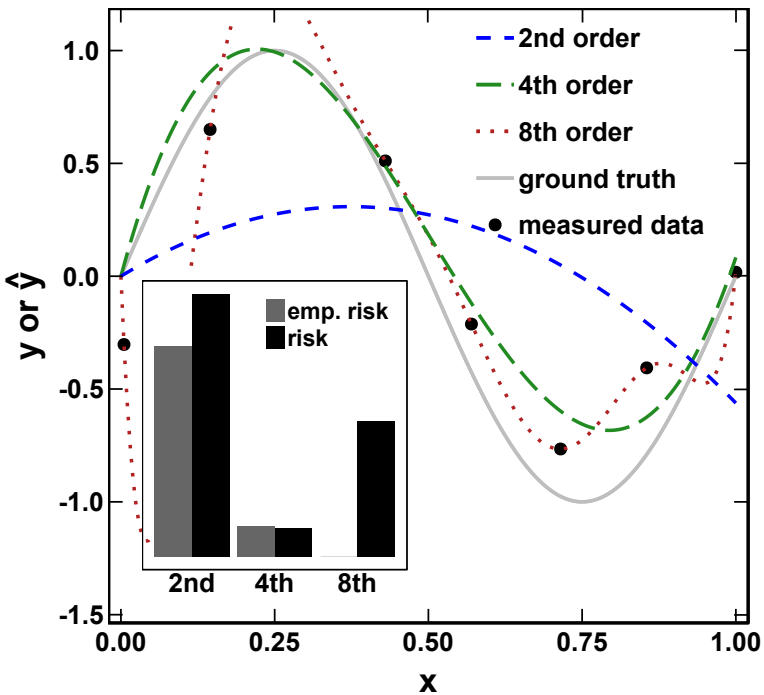

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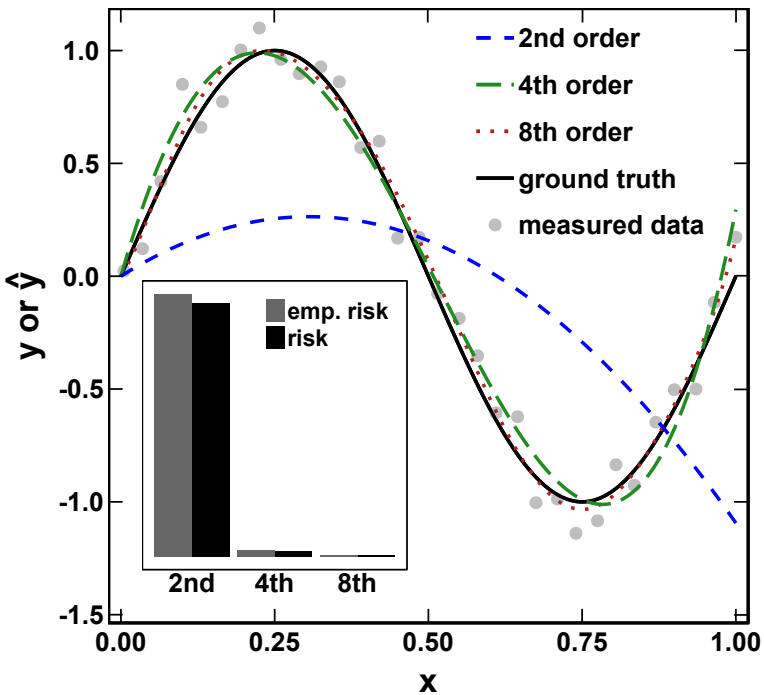
What happens if we add more data?



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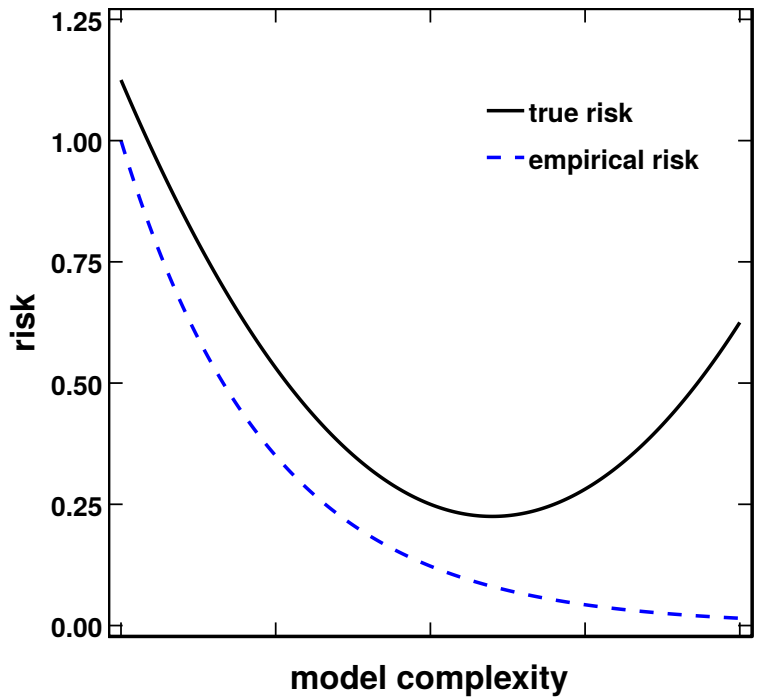
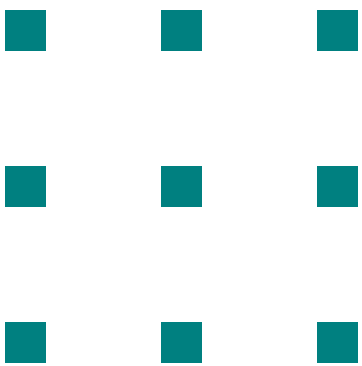
We cannot choose model complexity (hyperparameters, regularization) based on training data.

Cross-validation (and related techniques) must be used to compare models.

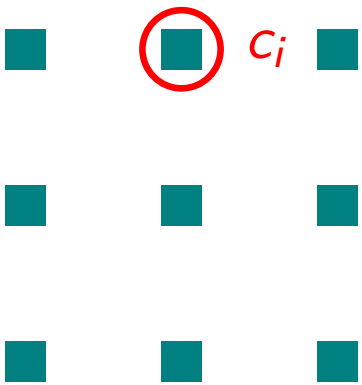


C4: Representing chemical systems



Chemical Space C_f

C4: Representing chemical systems



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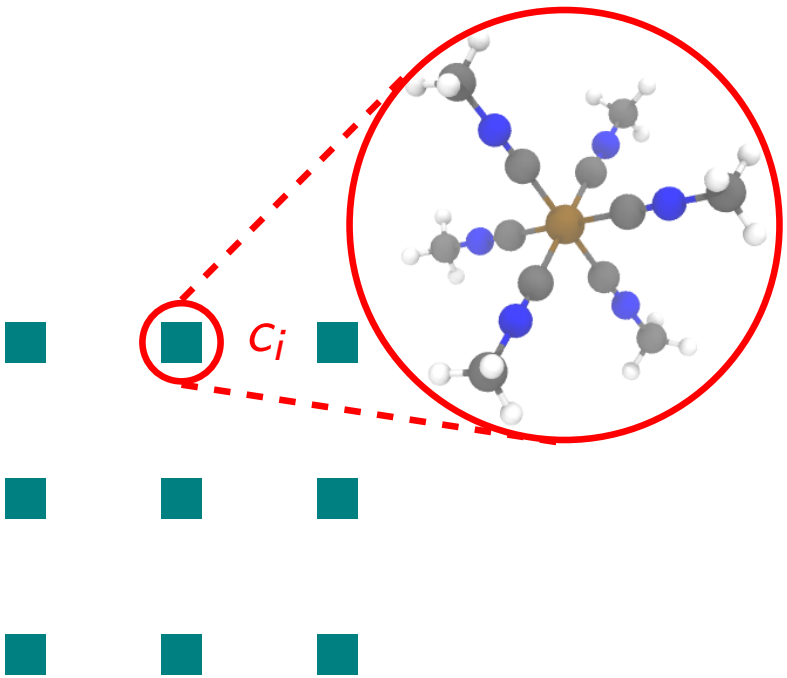

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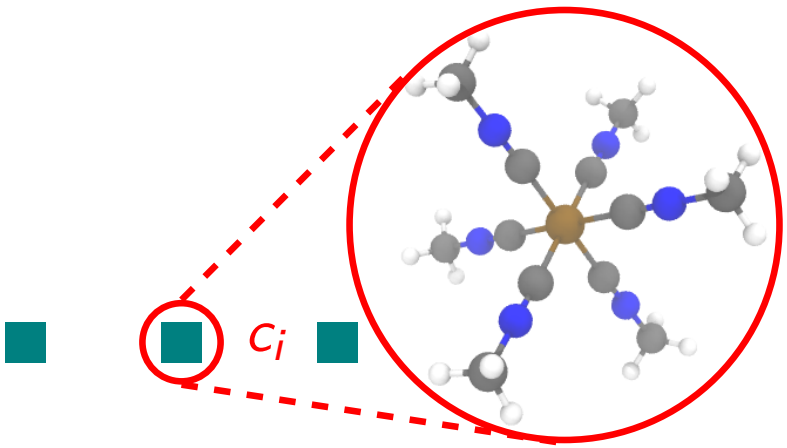

Chemical Space C_f

Descriptor Space $\mathcal{X} \subset \mathbb{R}^d$

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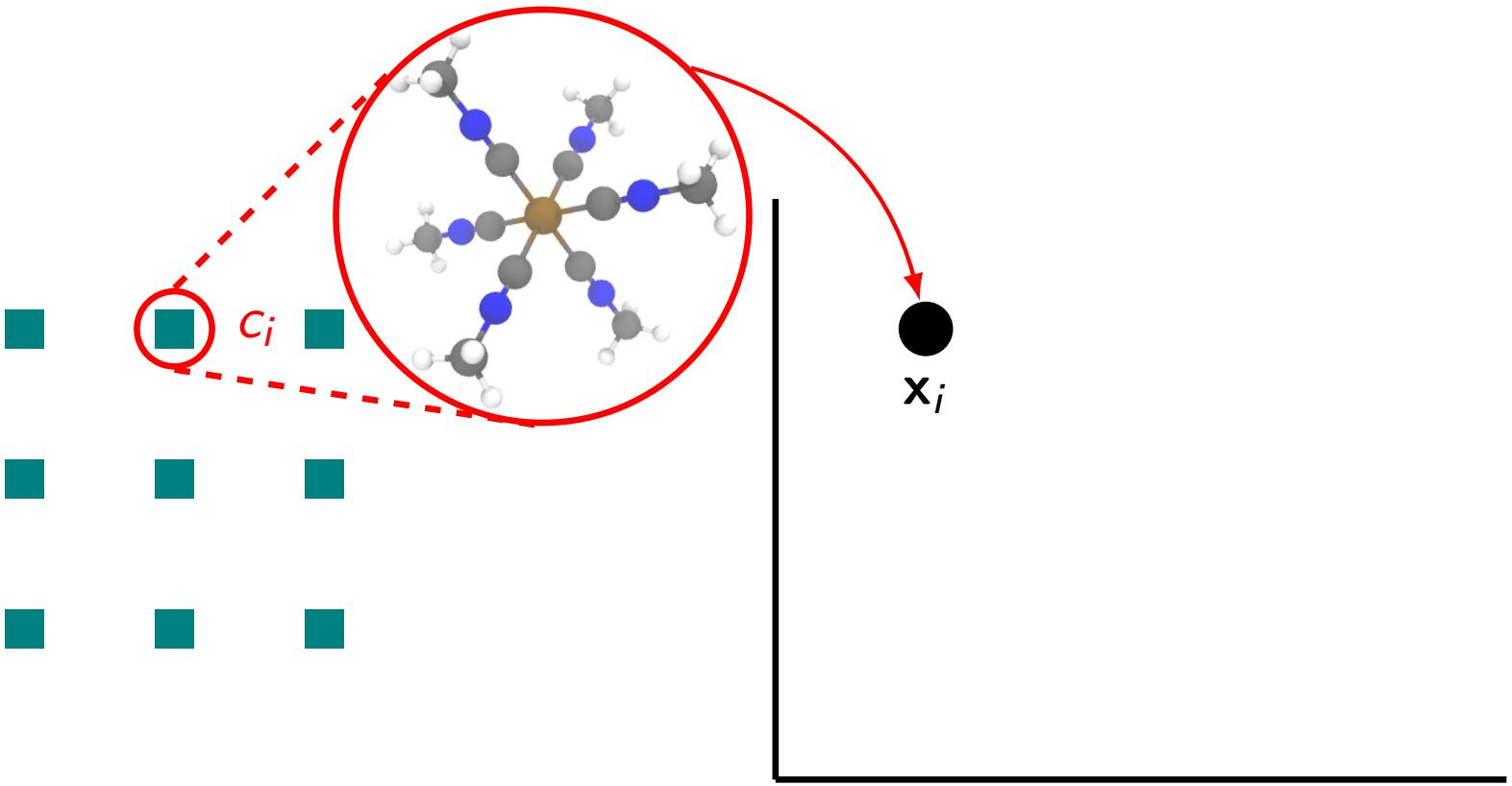

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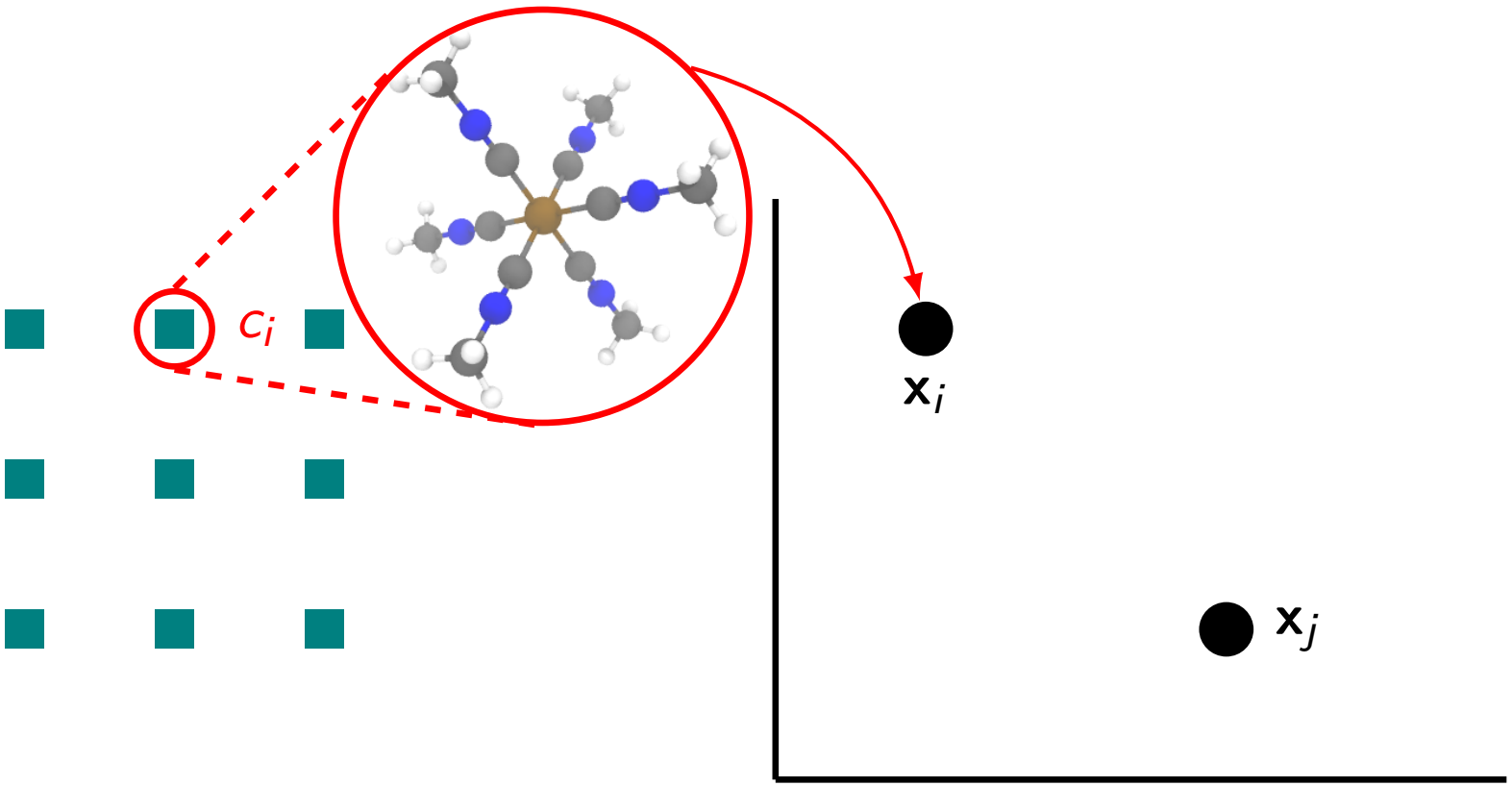

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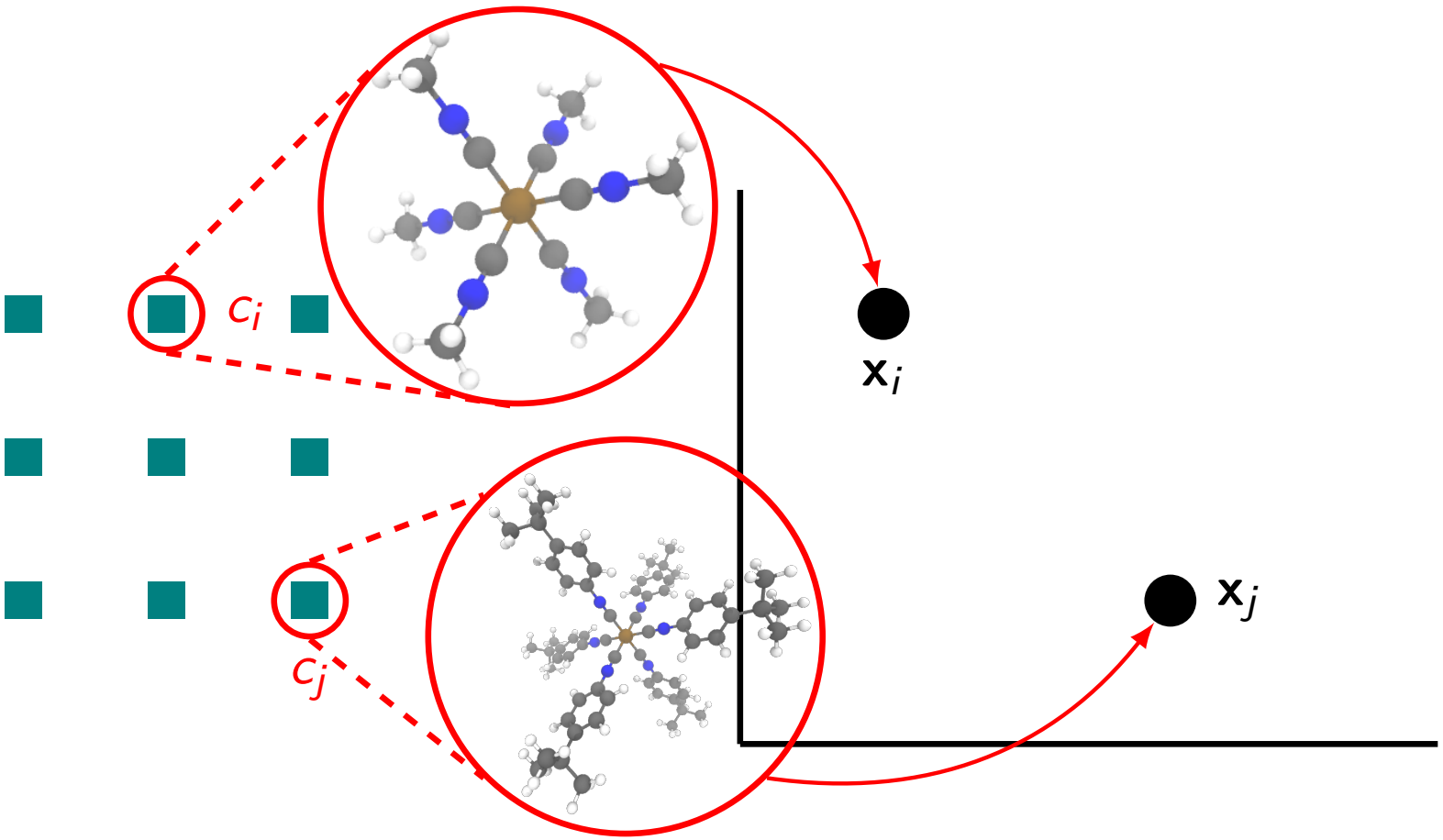

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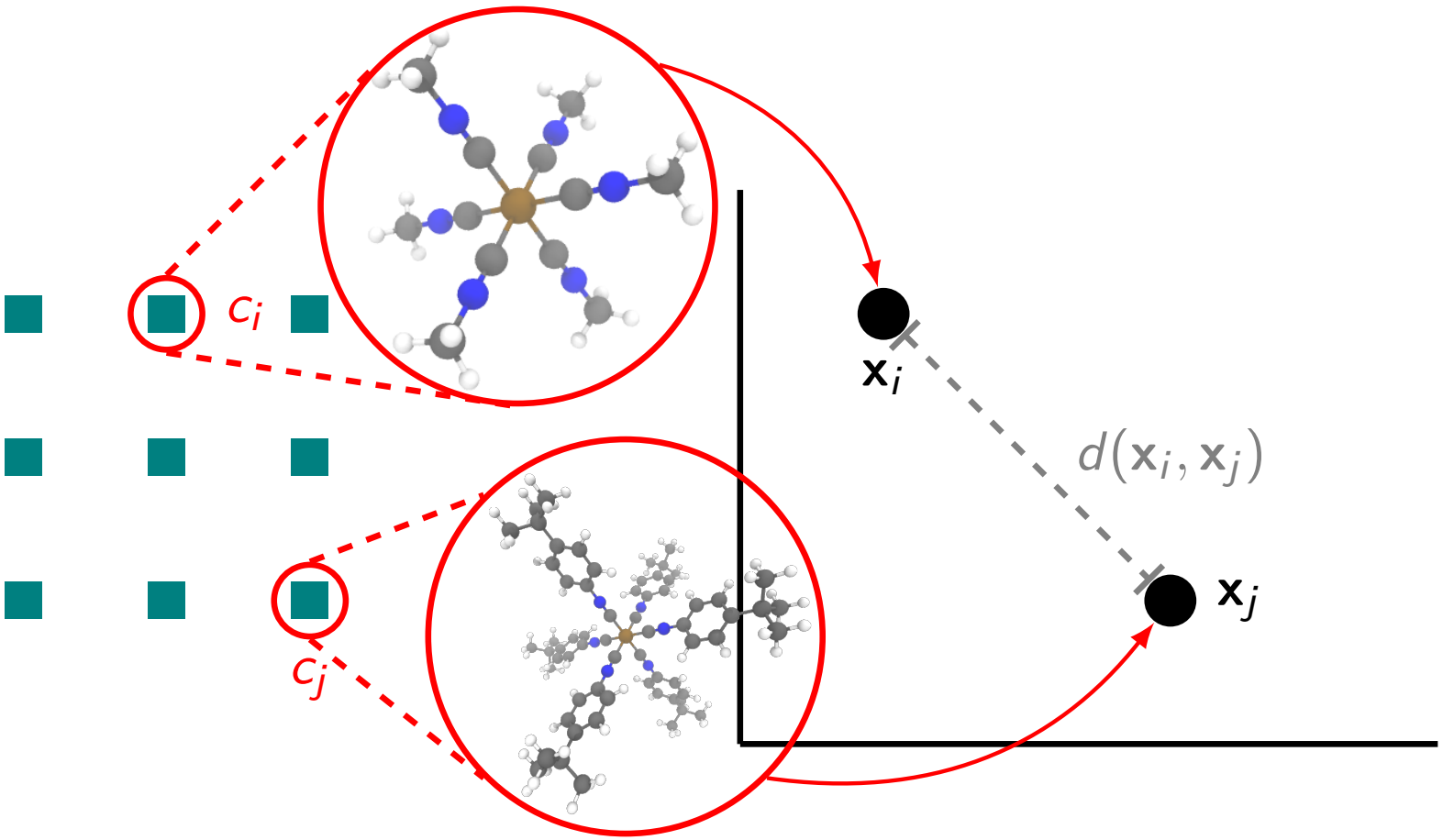

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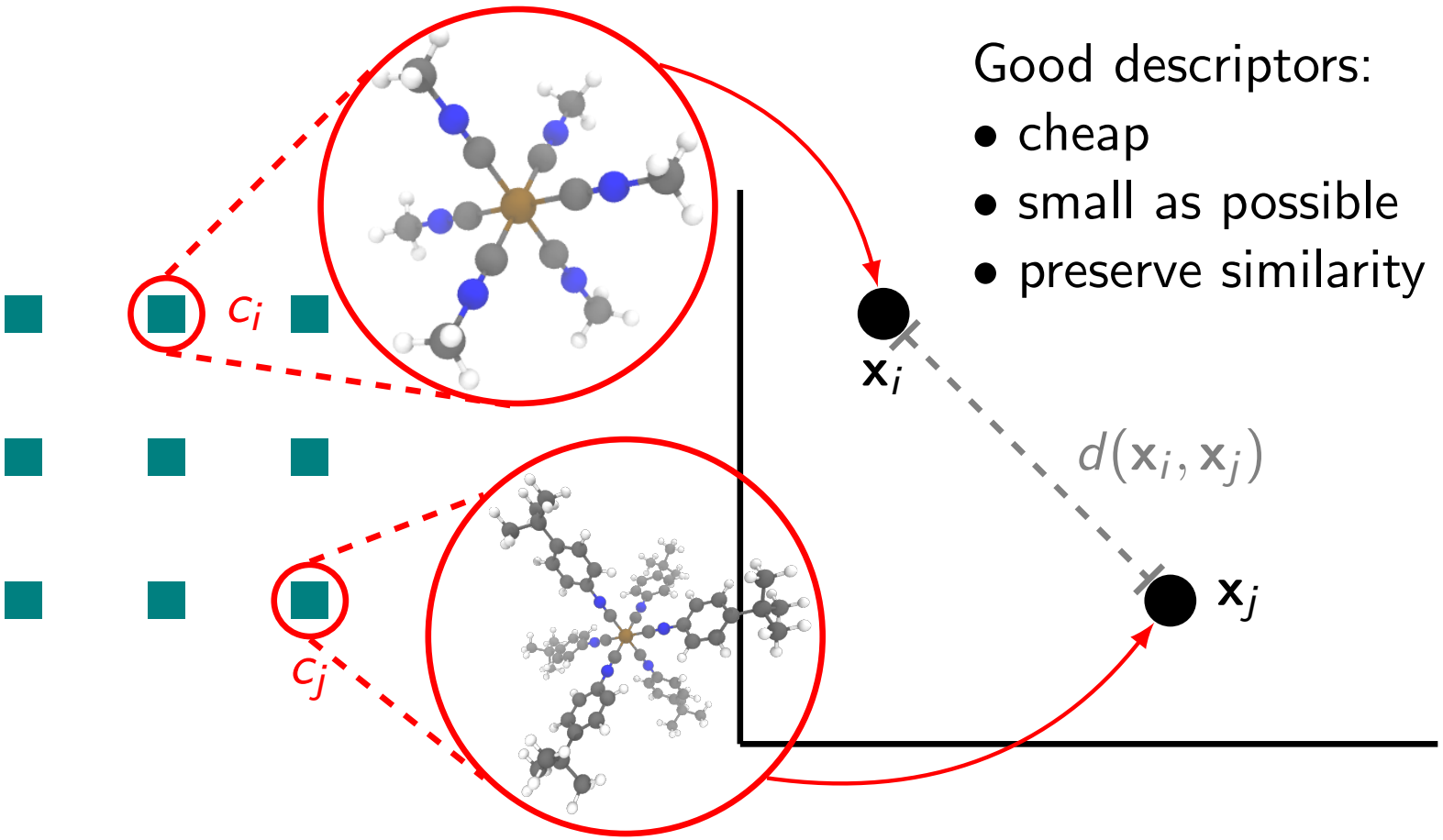

Good descriptors:

- cheap
- small as possible
- preserve similarity

Chemical Space C_f

Descriptor Space $\mathcal{X} \subset \mathbb{R}^d$

C5: How neural networks work

Simple neural networks can be understood as learned, continuous maps from the input space to a latent space, followed by linear regression

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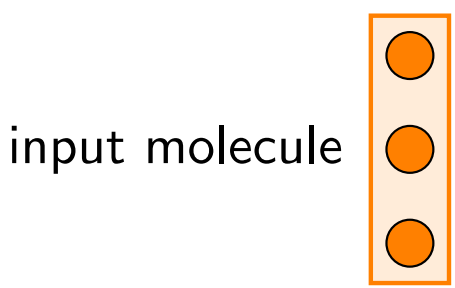

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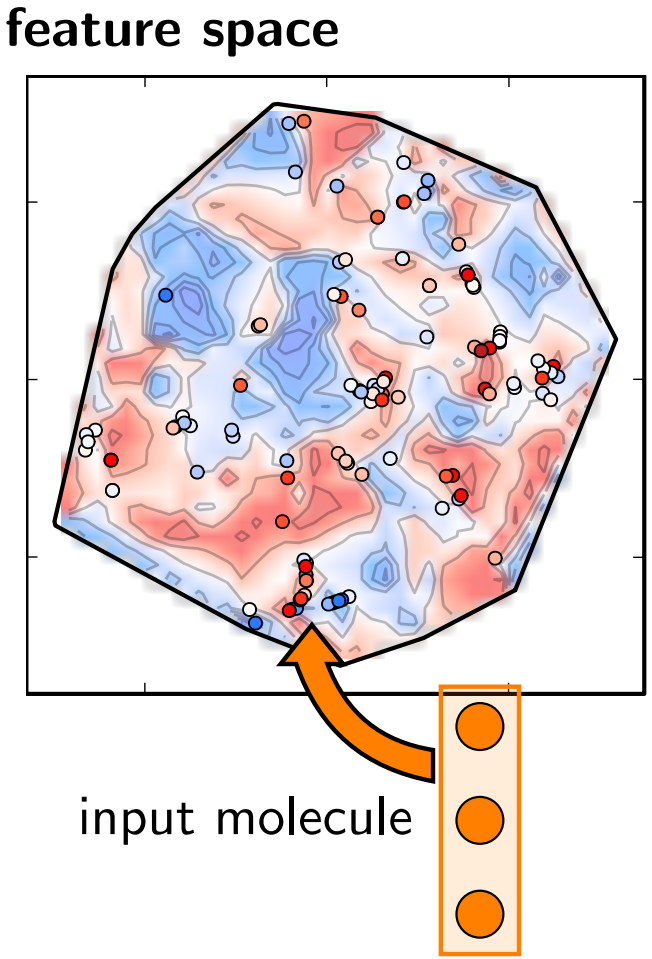

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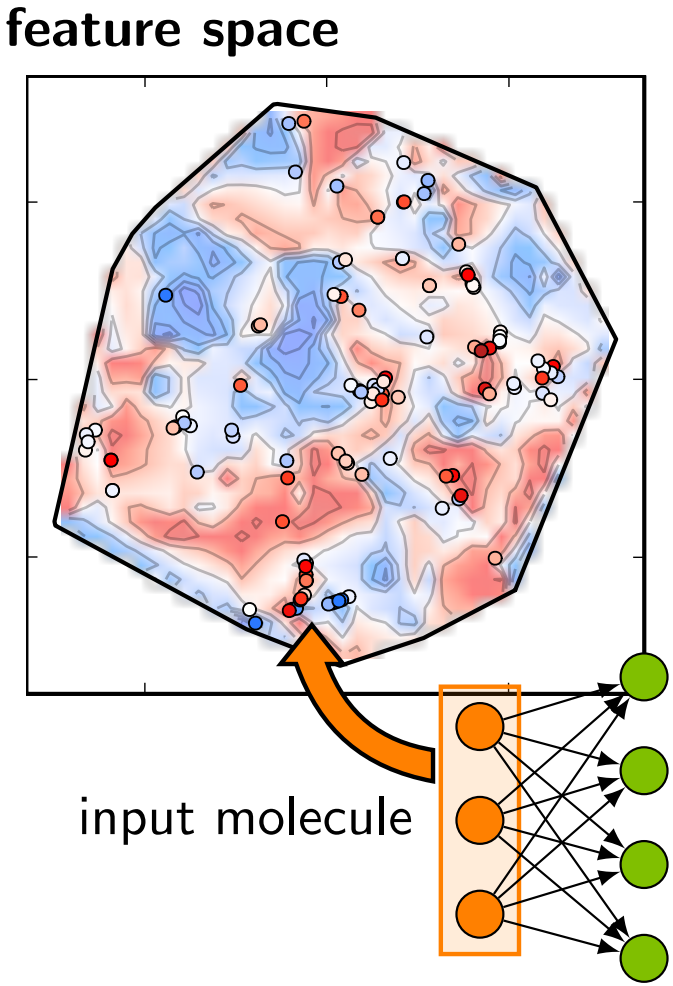

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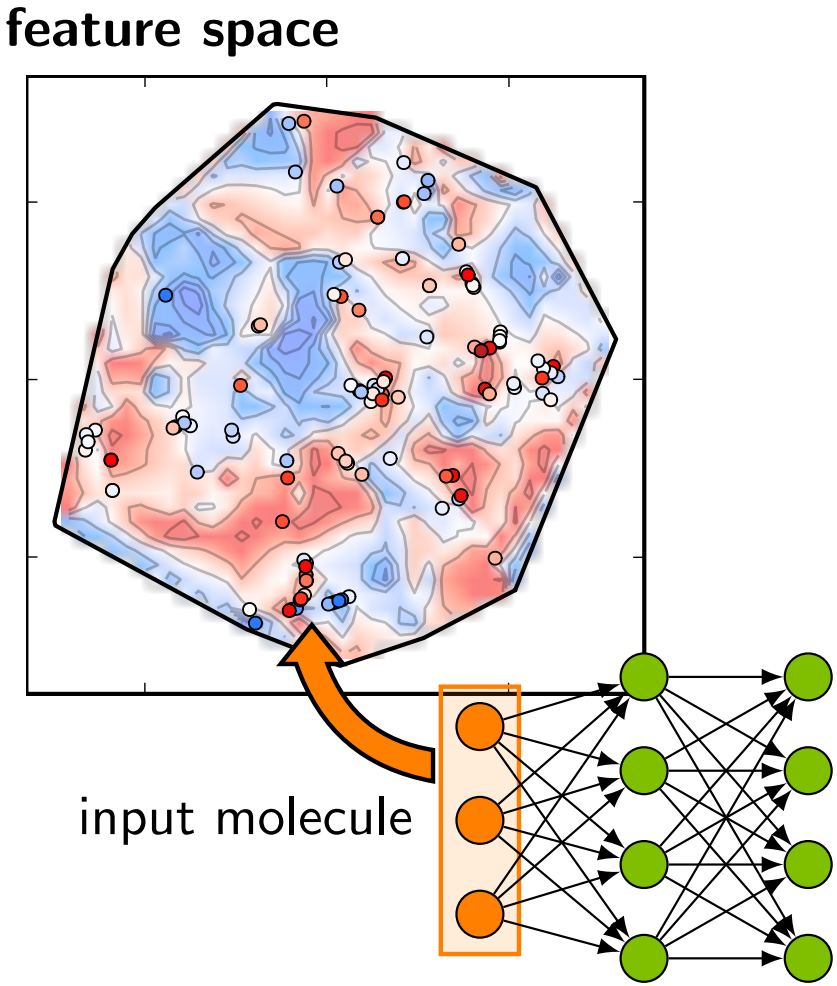

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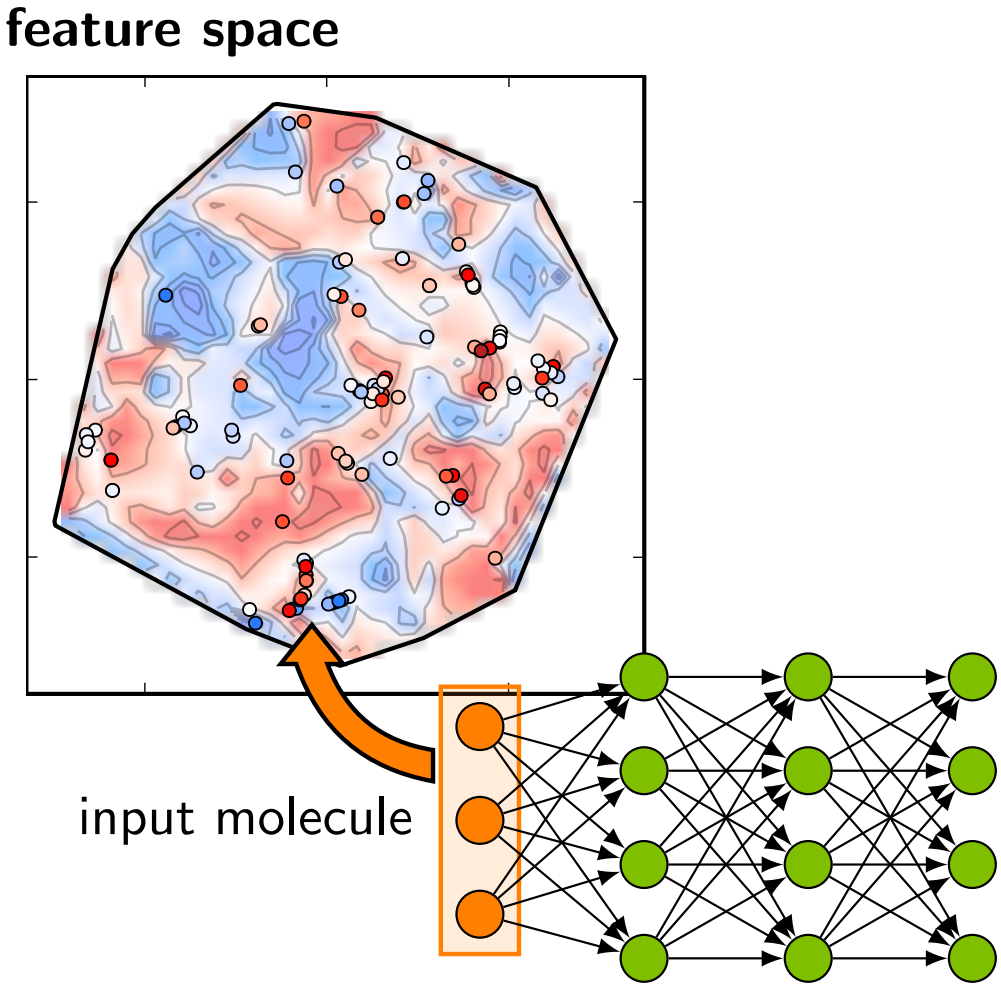

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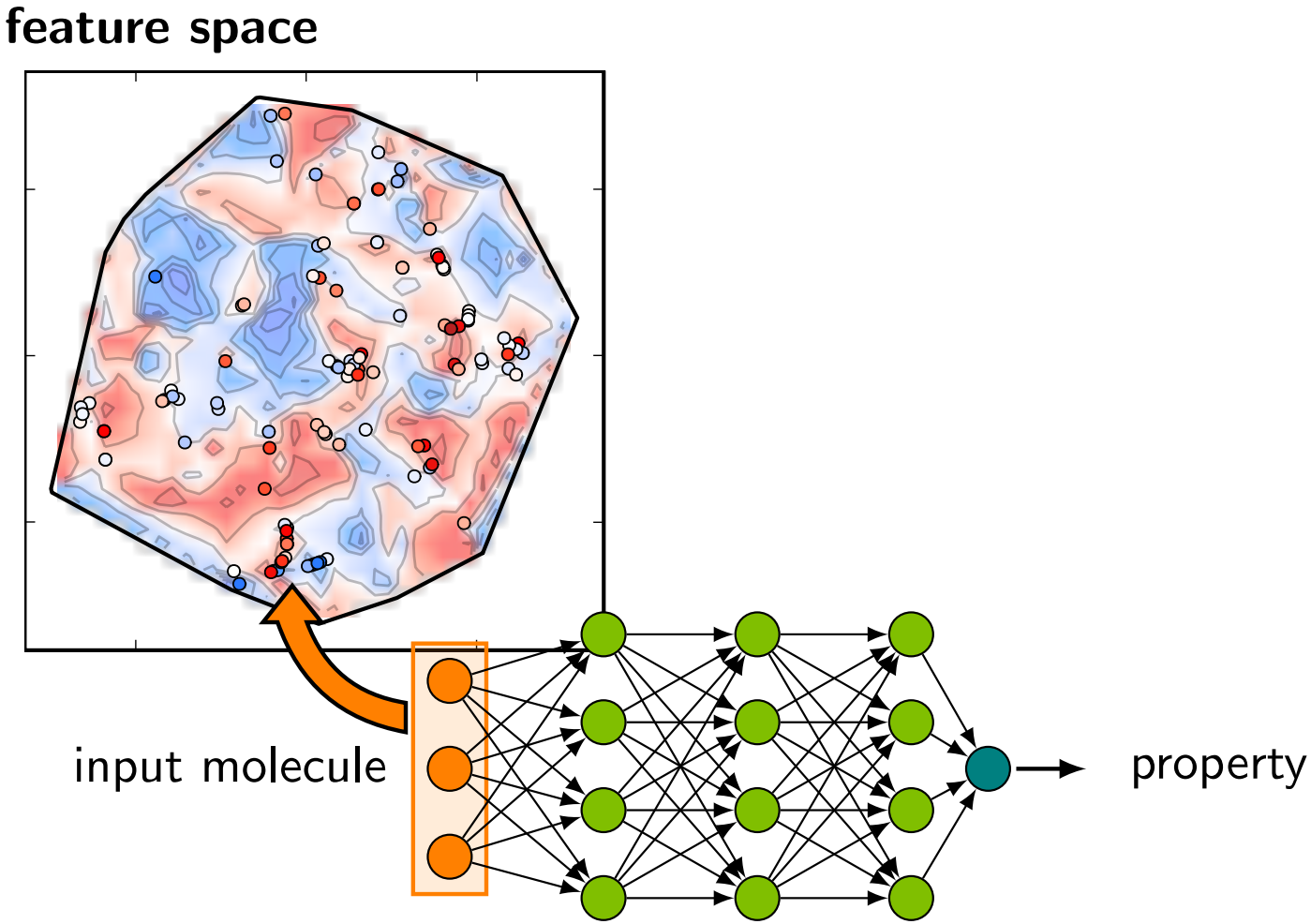

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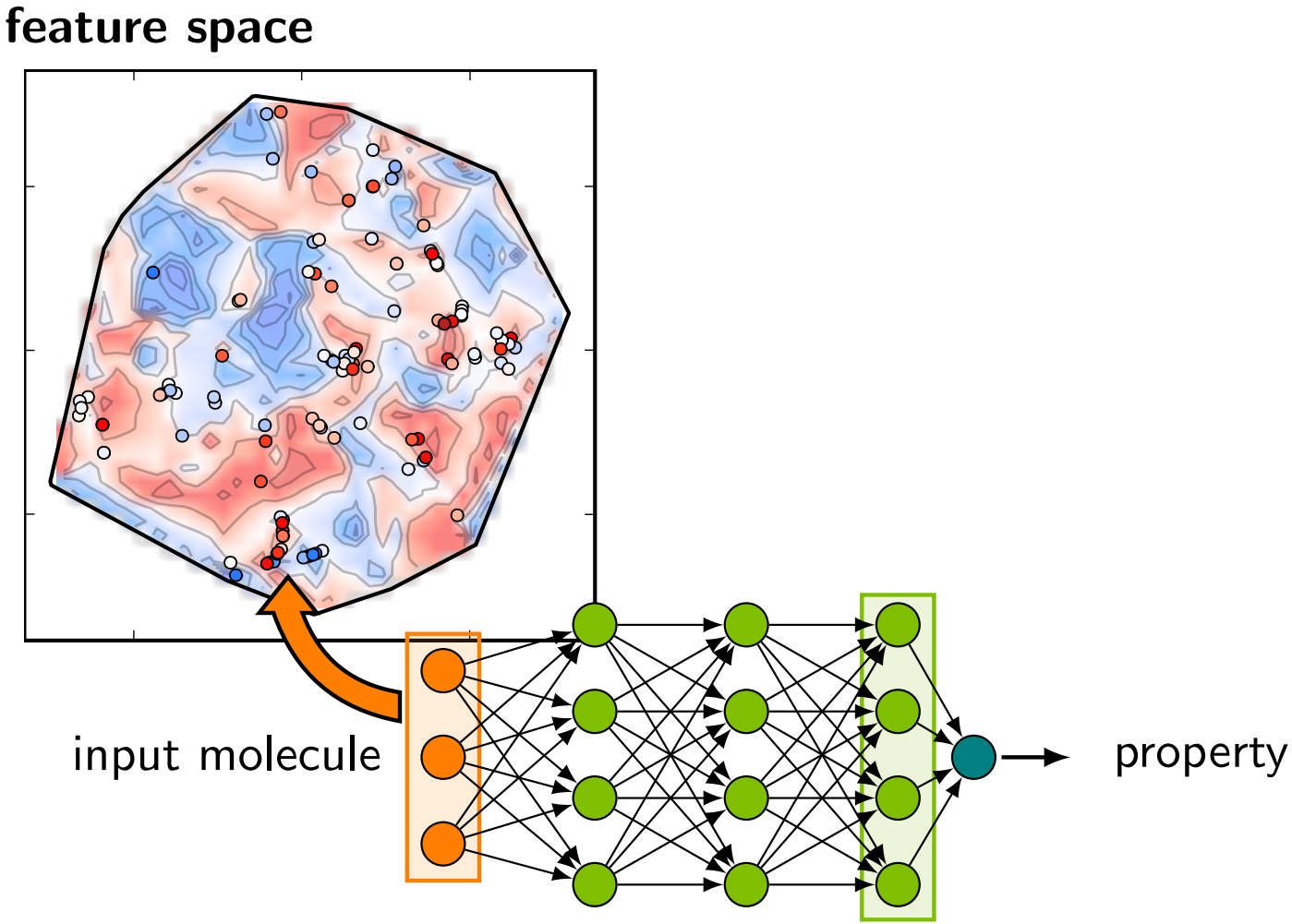

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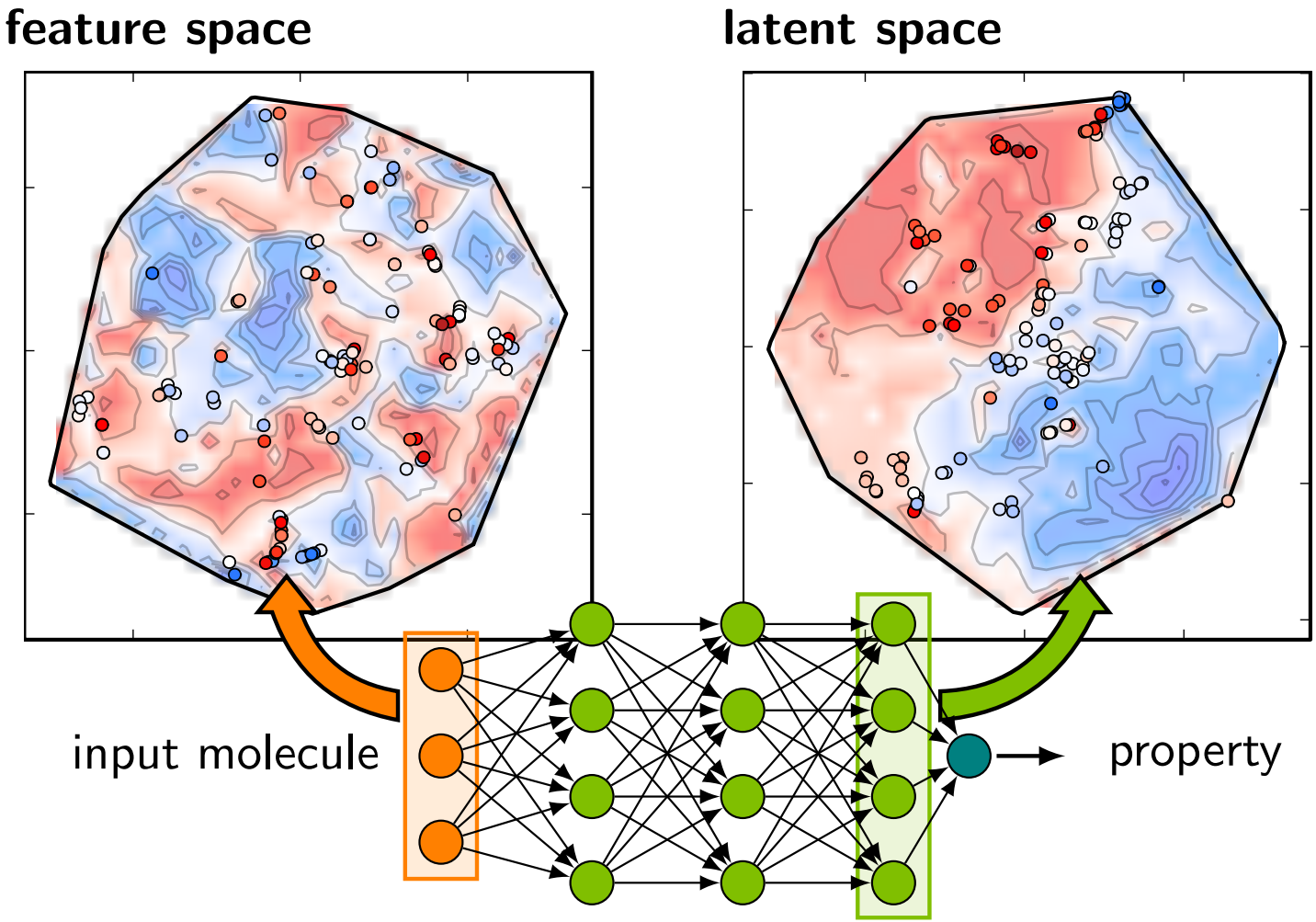

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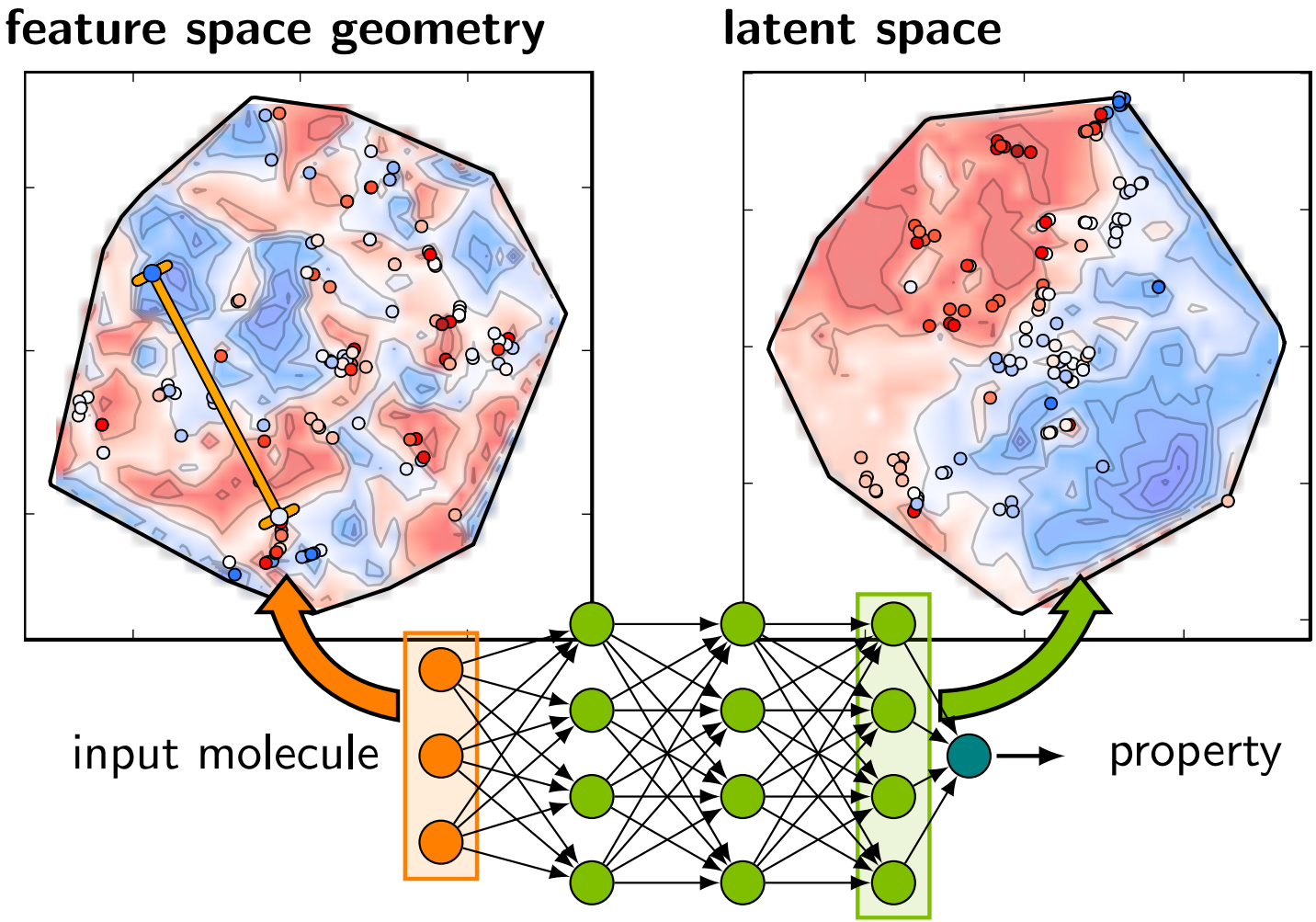

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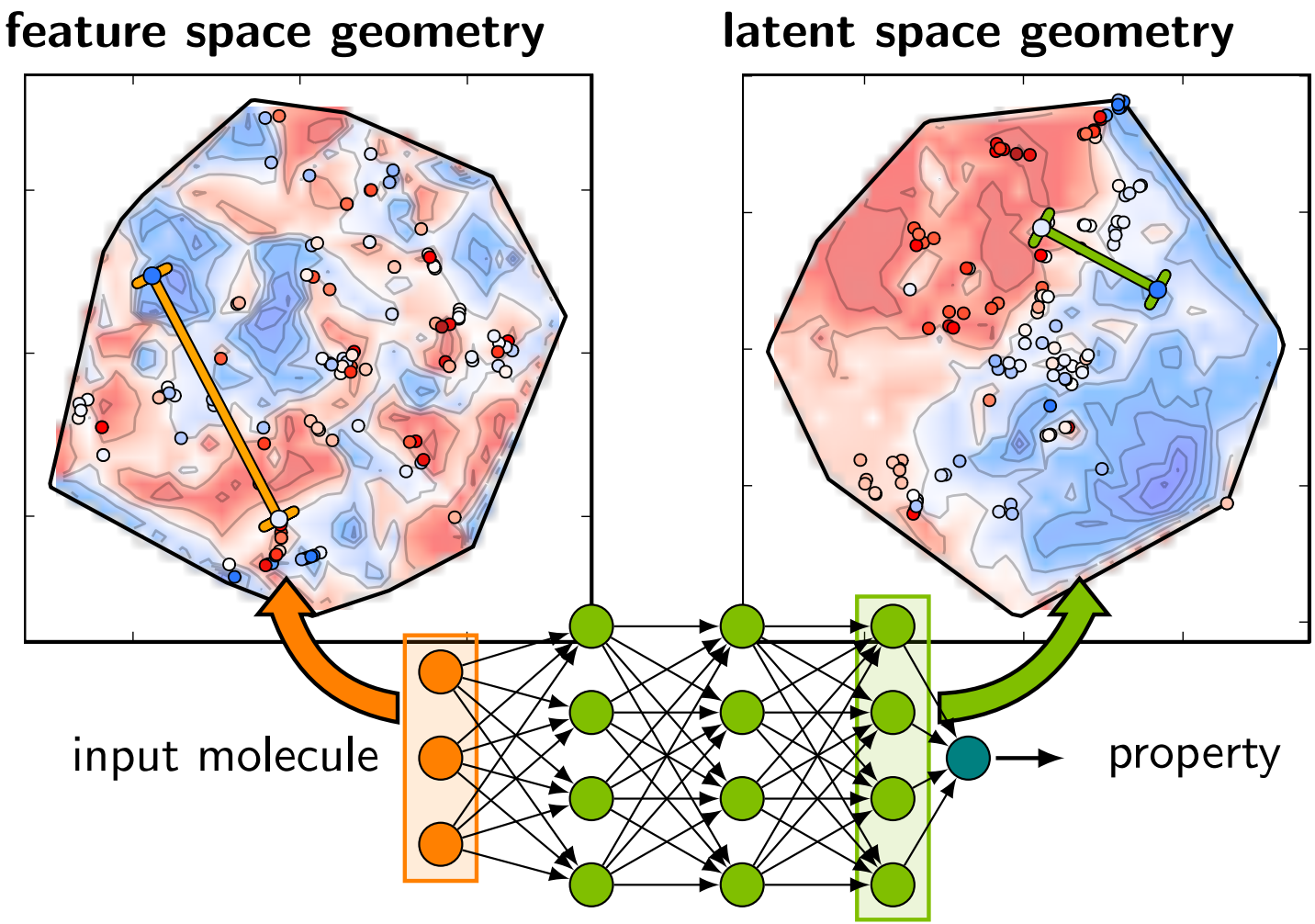

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Final thoughts

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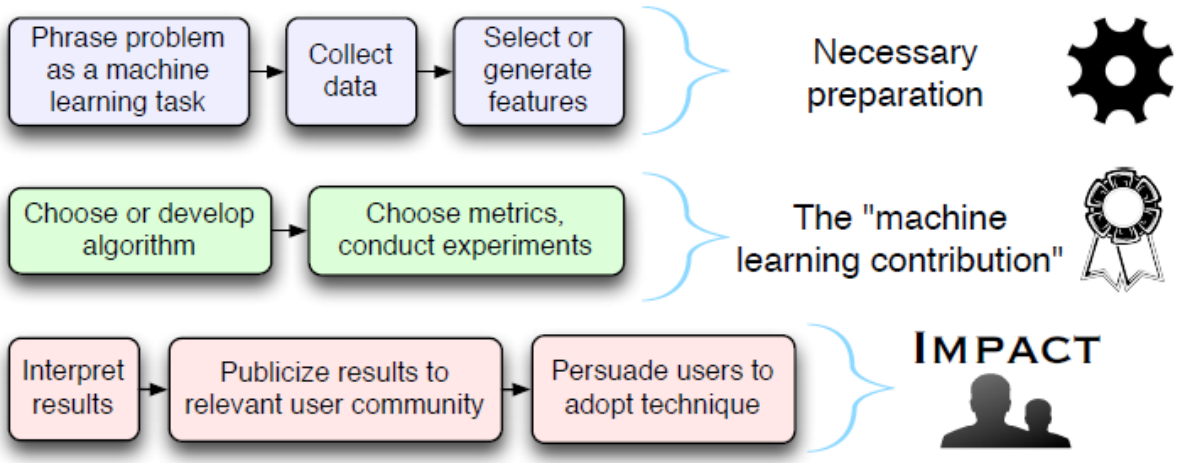

Wagstaff, K., "Machine Learning that Matters", ICML 29, 16(7):529–536, 2012

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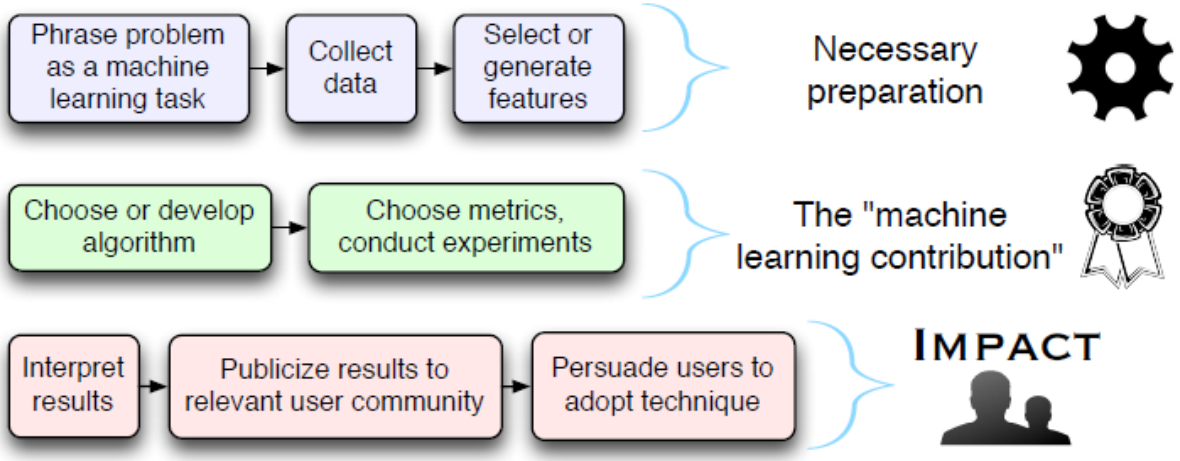
It is increasingly important to be literate about ML concepts. Even if/when the hype lessens, ML tools will continue to have a large impact on our science.



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Conversely, there is a growing need for domain experts to engage and derive impact from advances in ML, and you have a lot of value to contribute to interpreting and exploiting the results.