ML for inorganic molecular design: descriptors and similarity in transition metal chemical space

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[1] Department of Chemical Engineering, Massachusetts Institute of Technology

255th ACS National Meeting, New Orleans

03.19.18

Data-driven molecular design

Machine learning is transforming how we design new materials...

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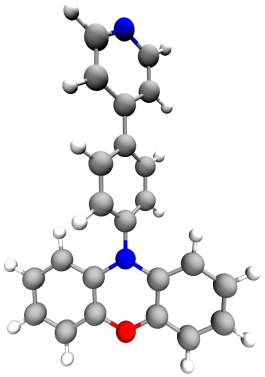

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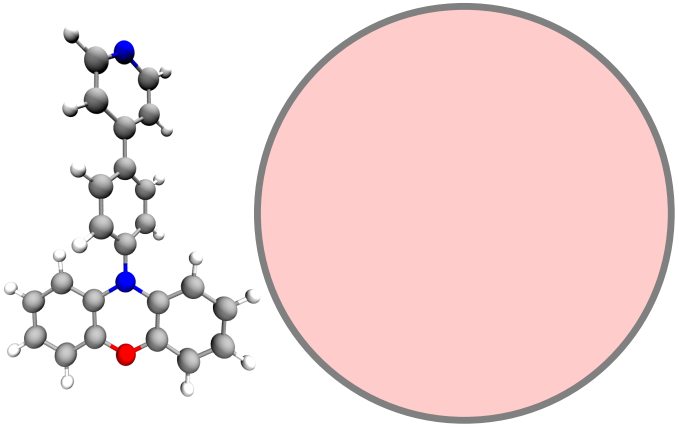

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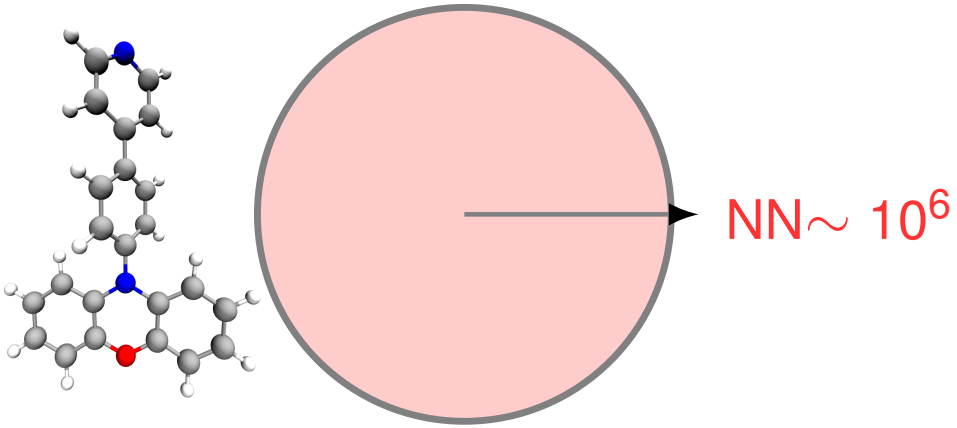

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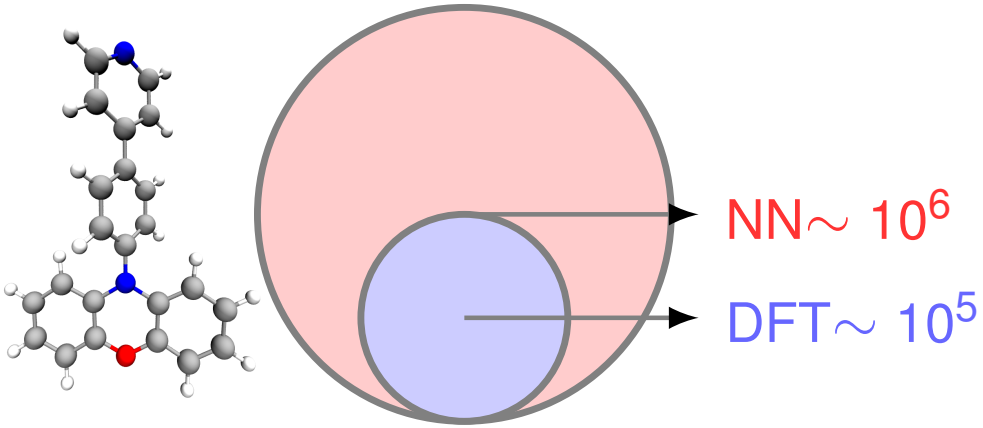

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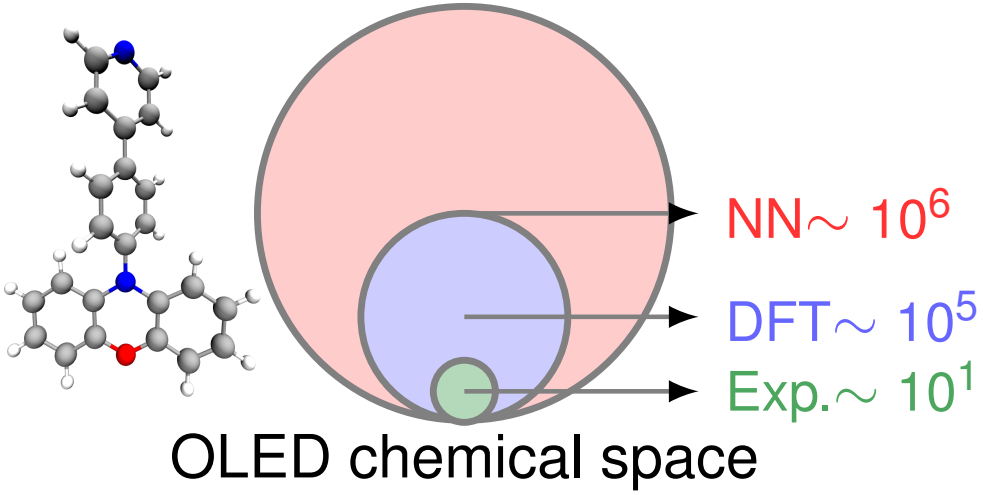

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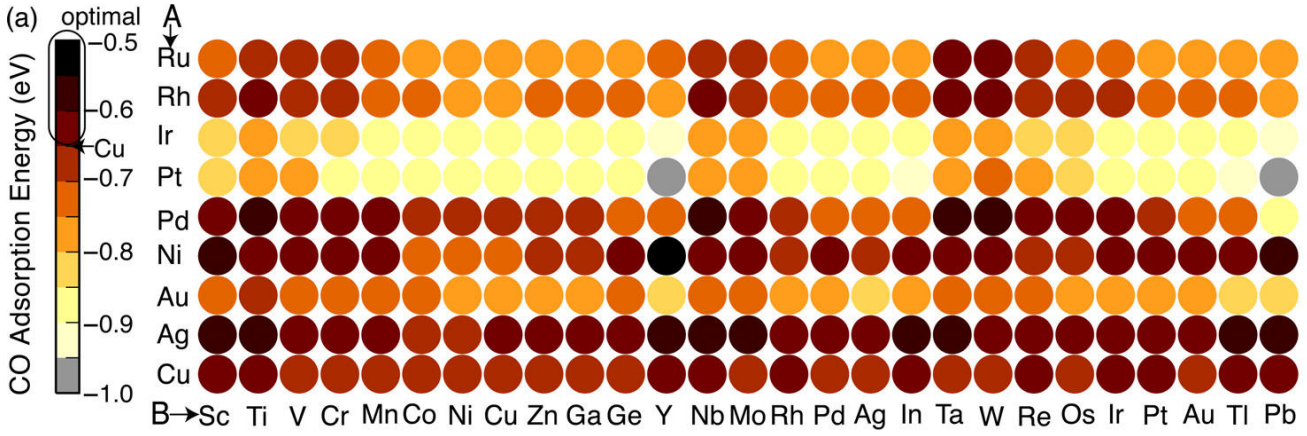

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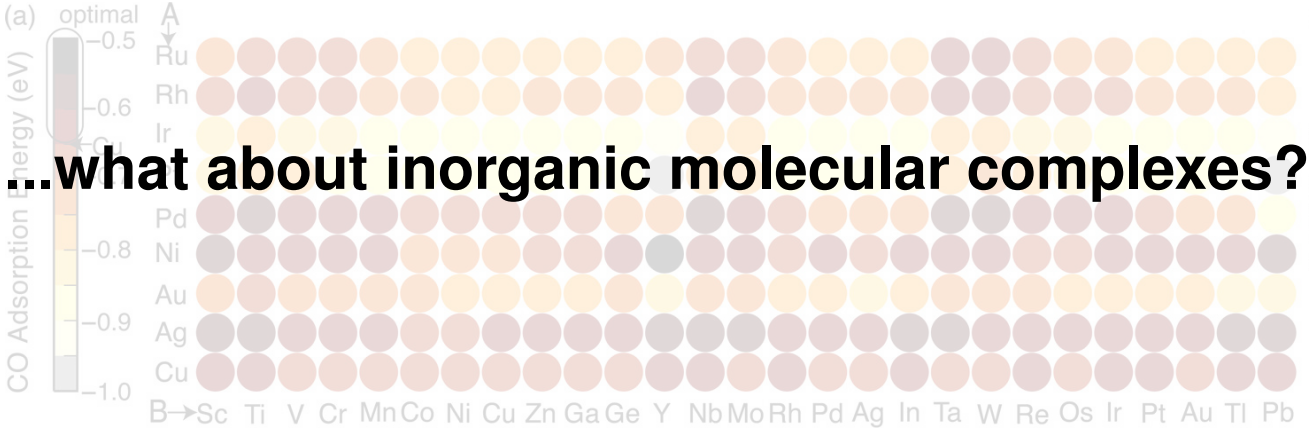

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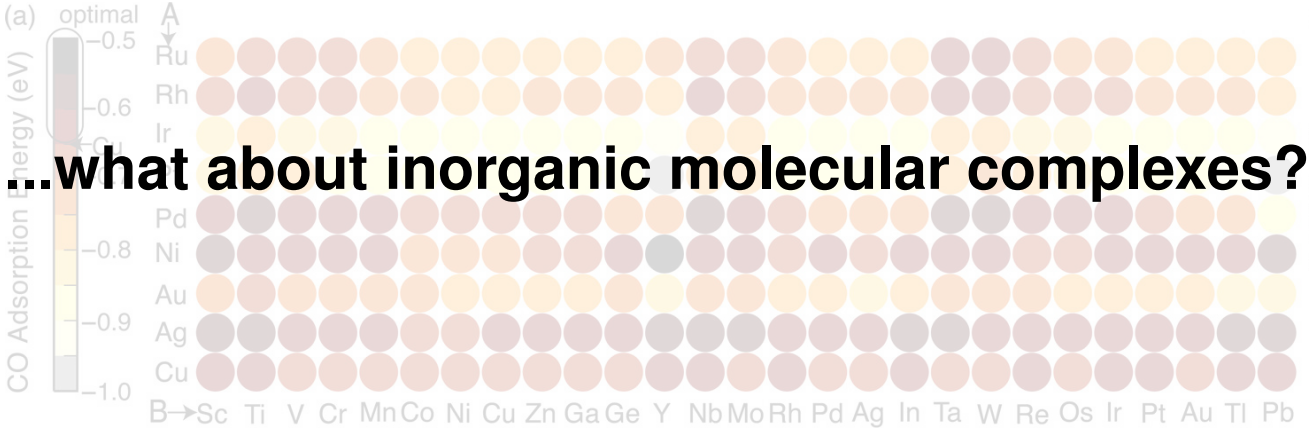

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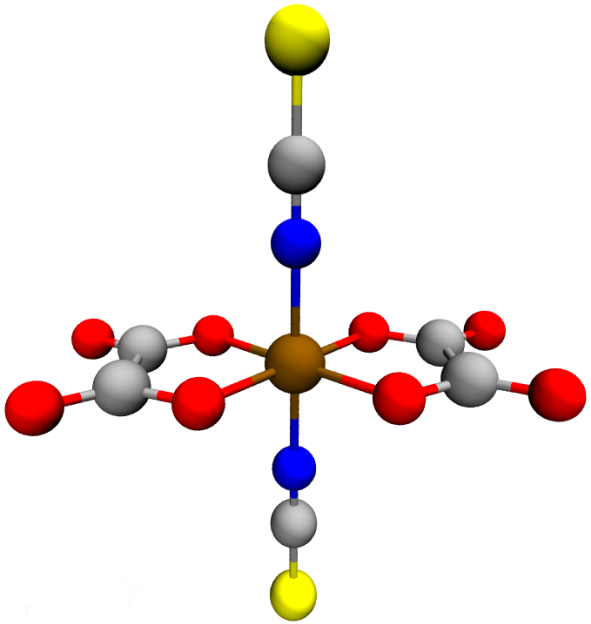

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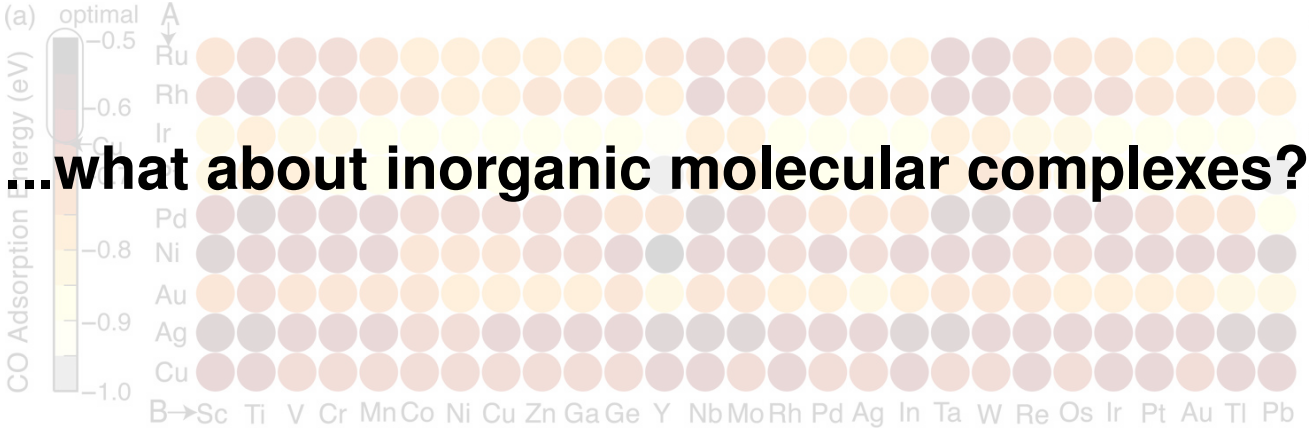

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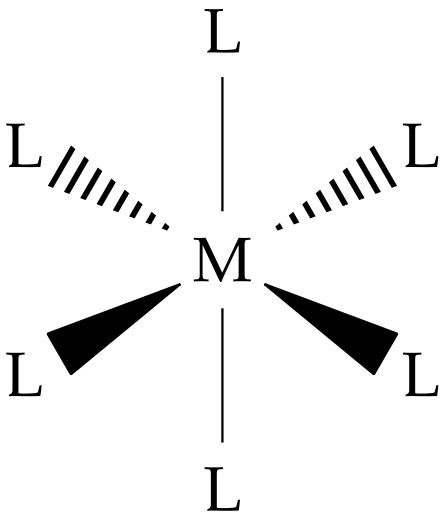

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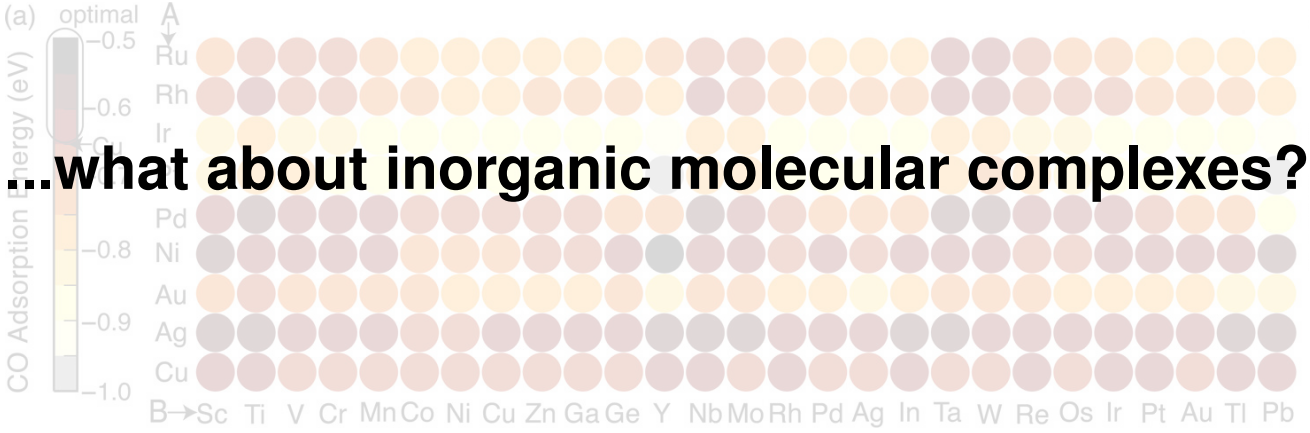

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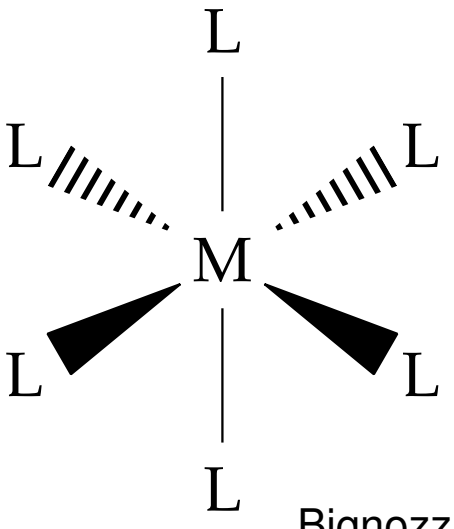

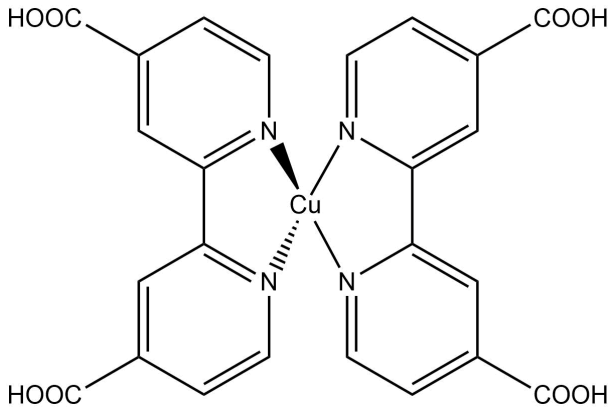

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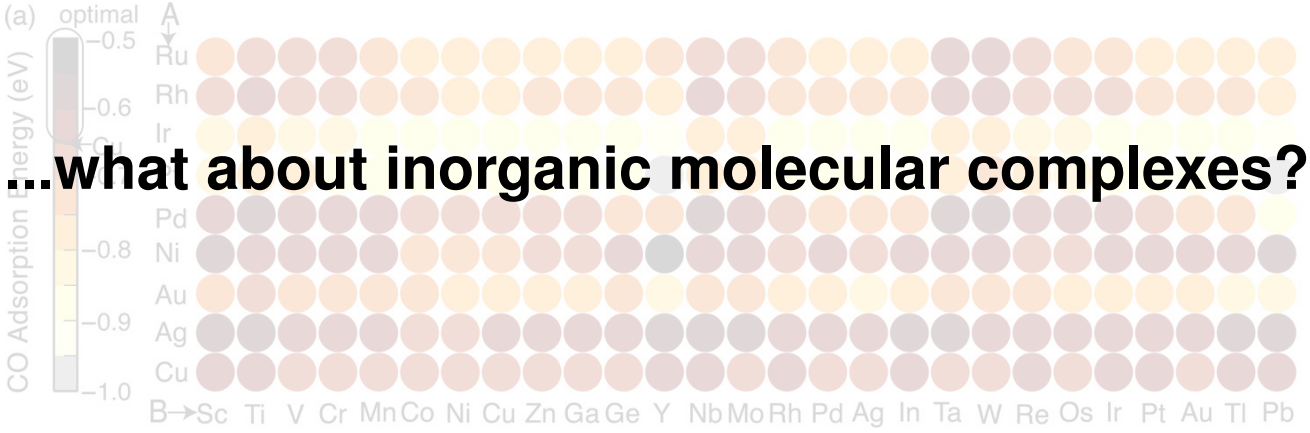

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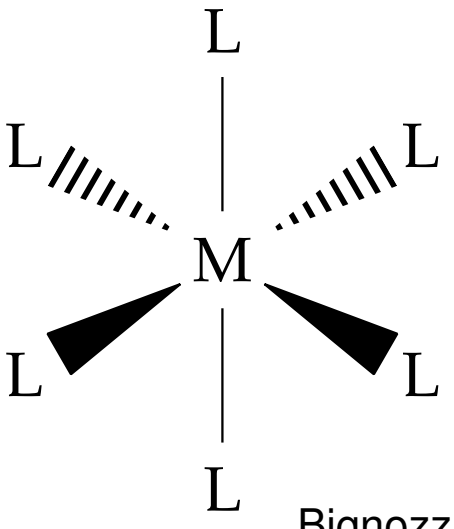

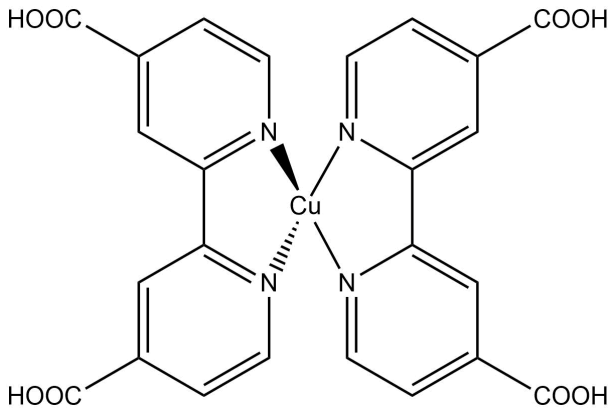

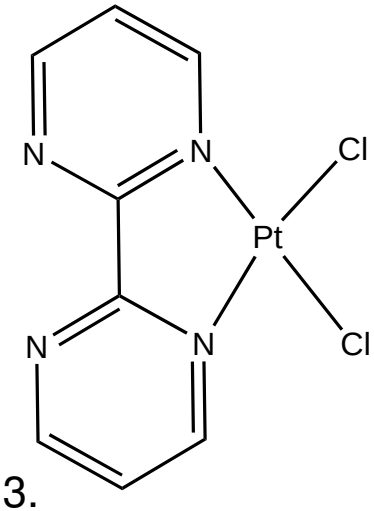

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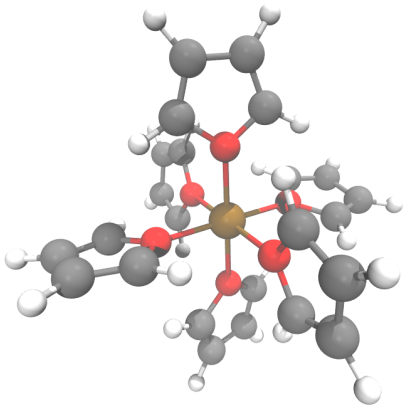

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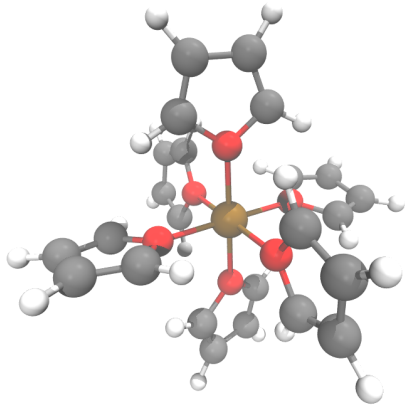

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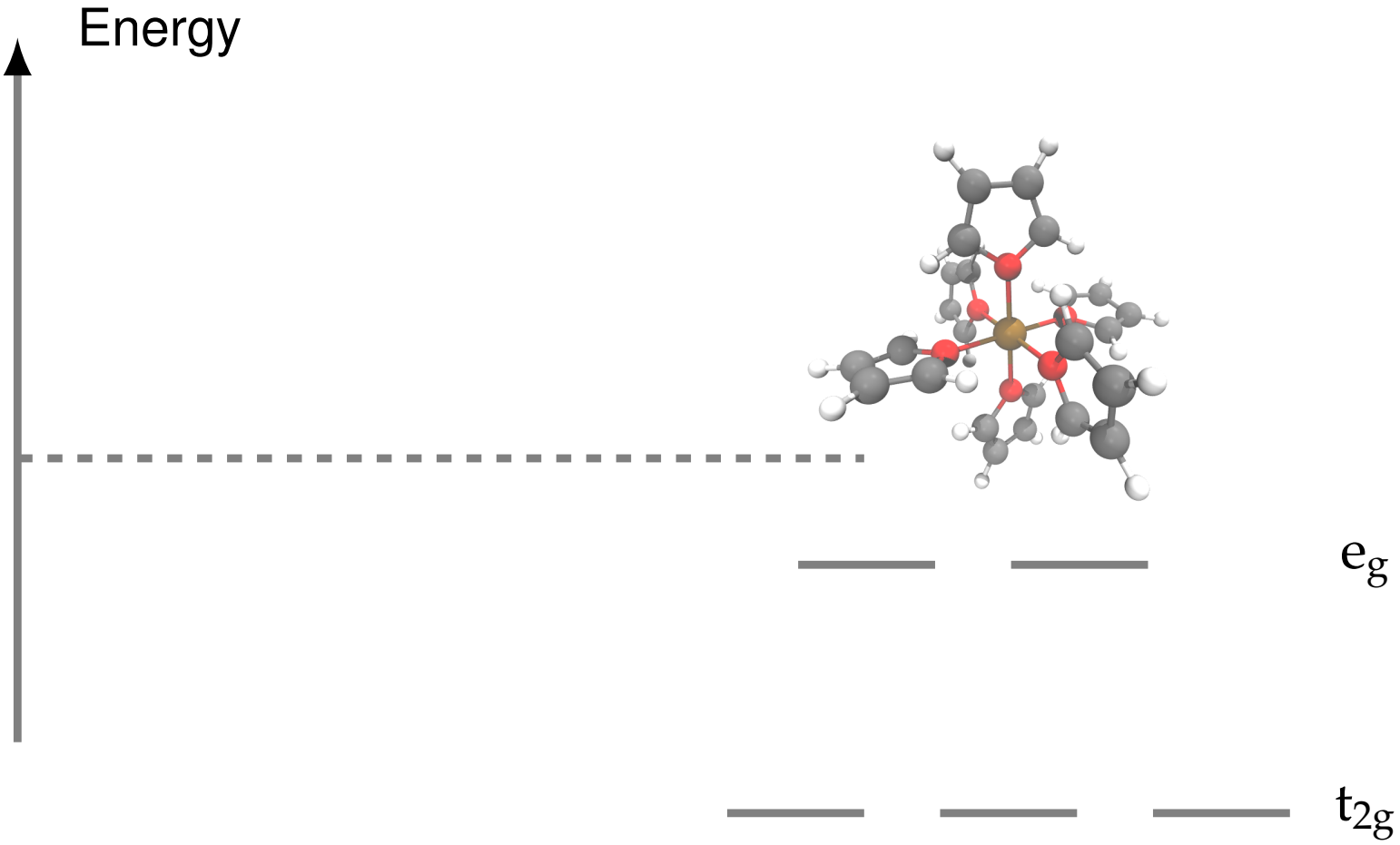

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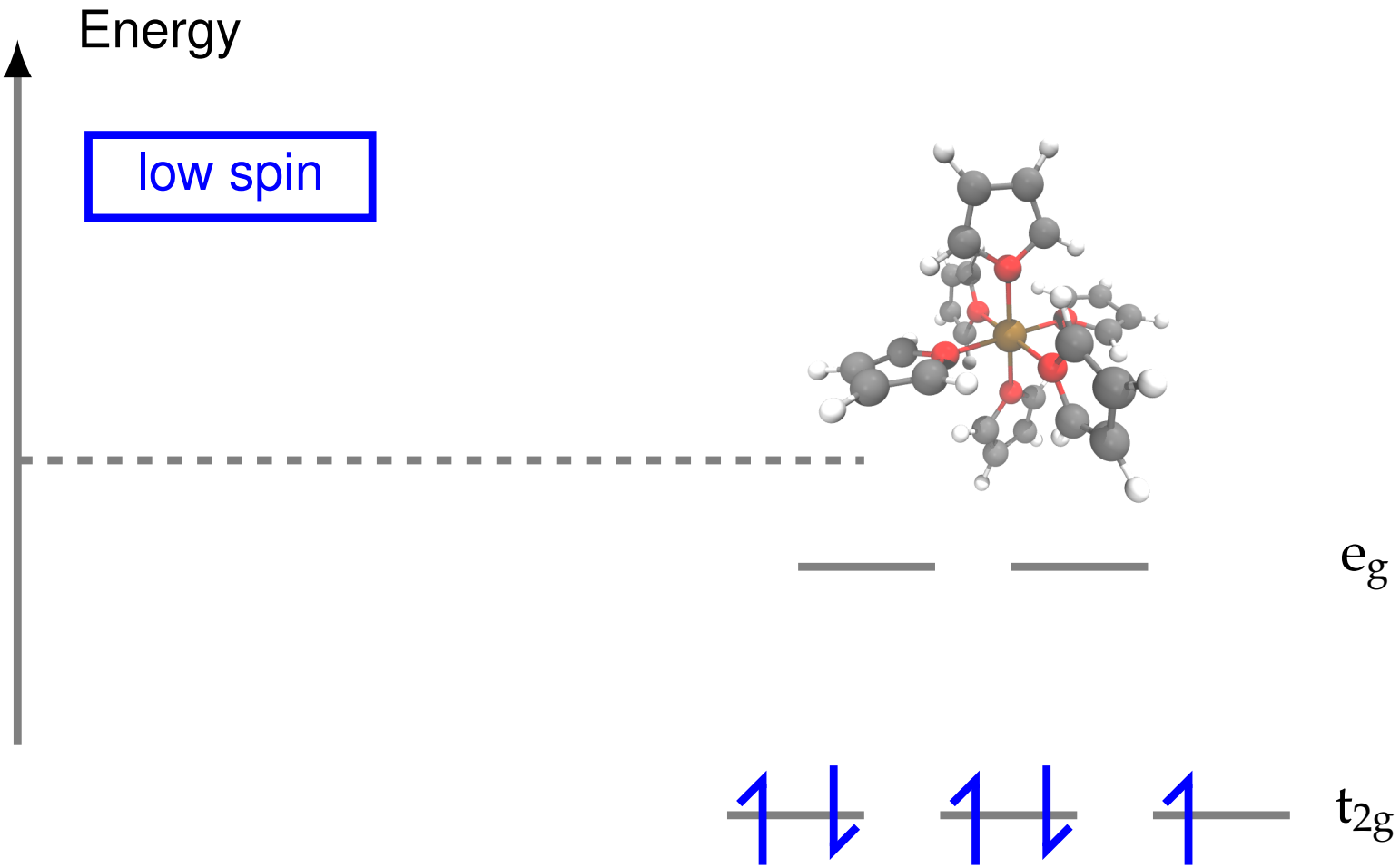

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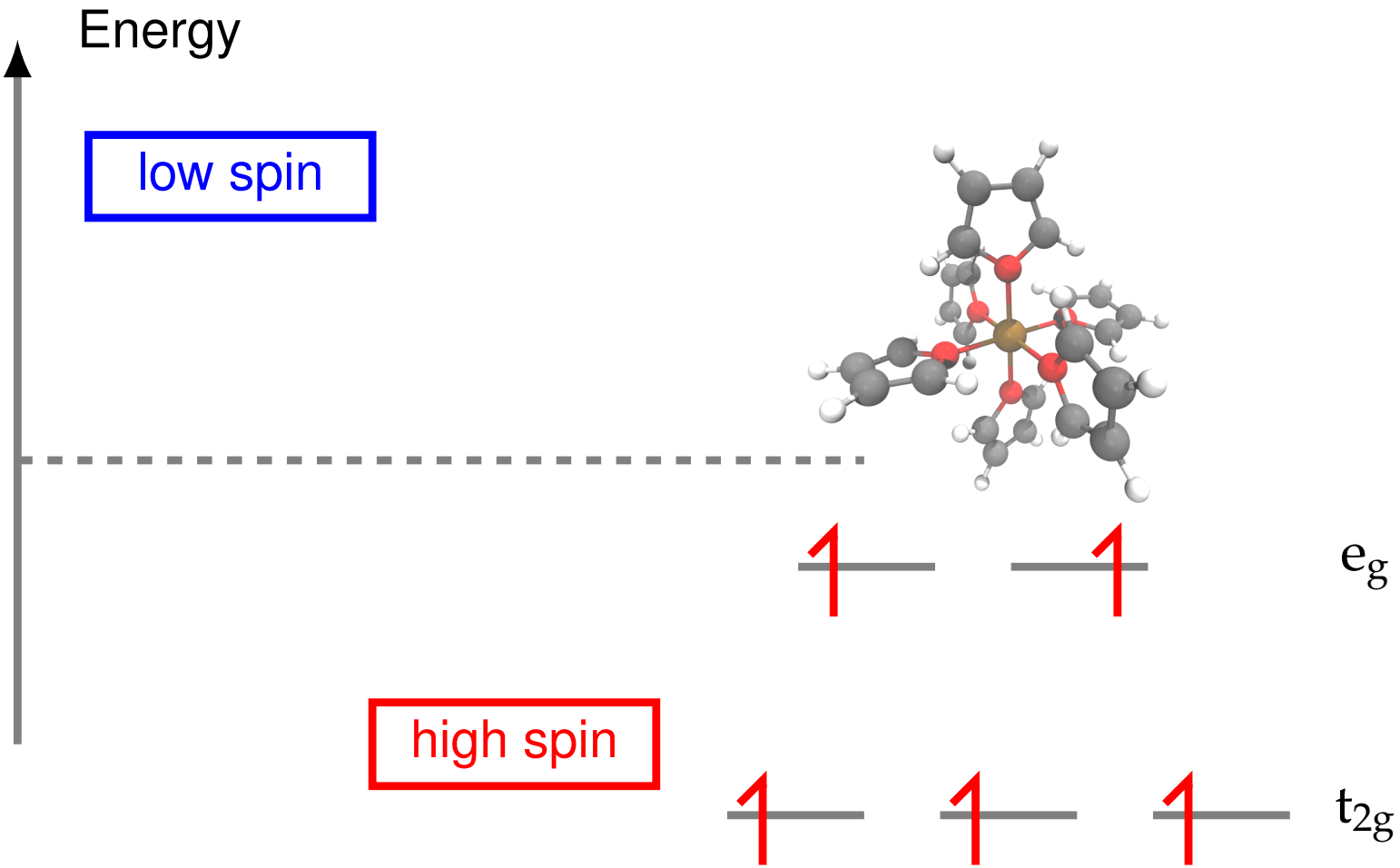

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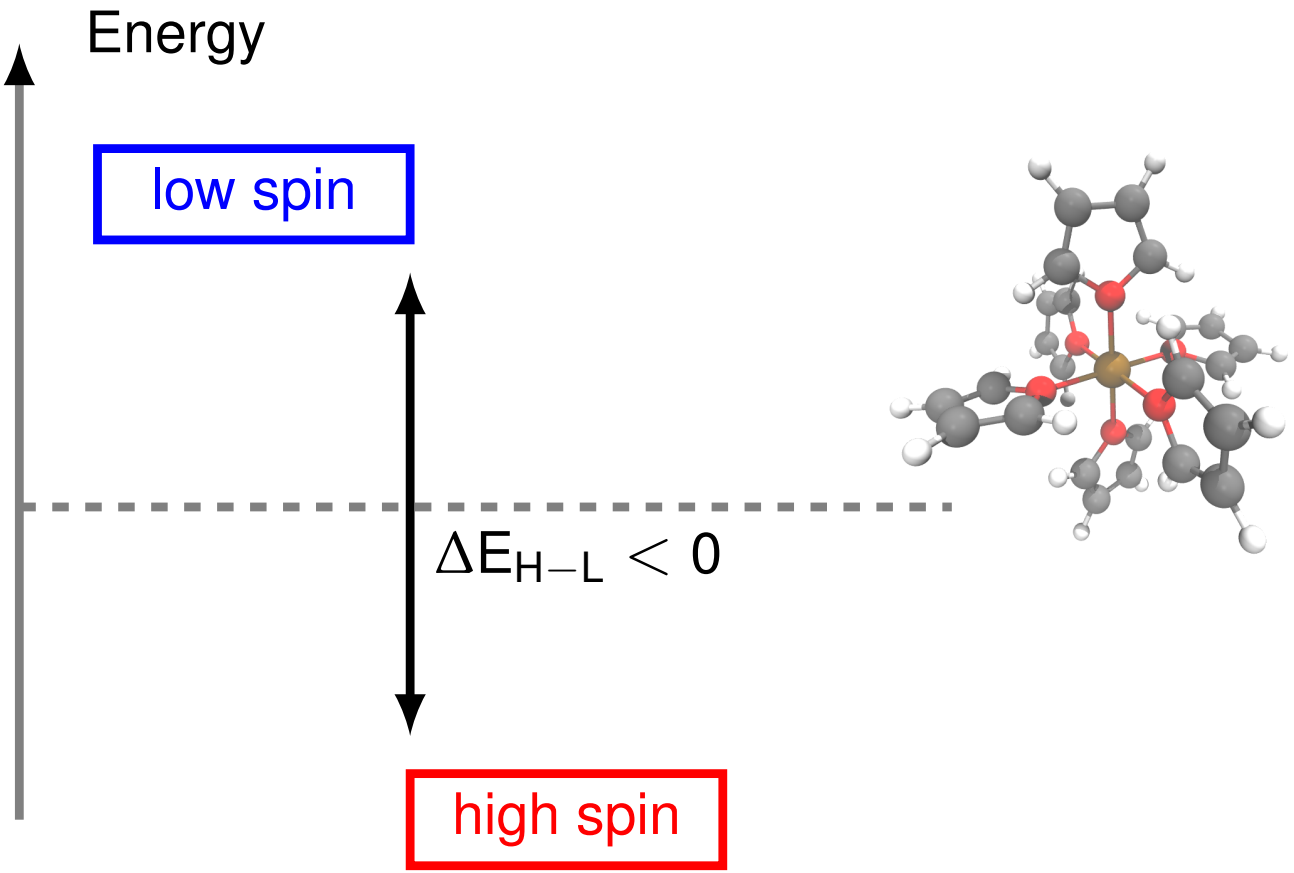

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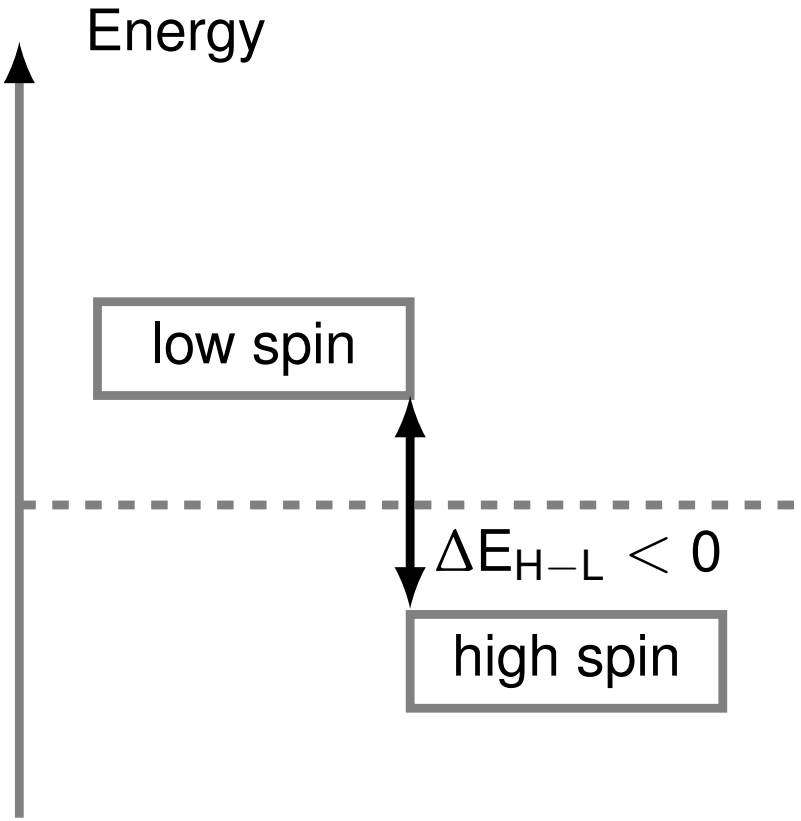

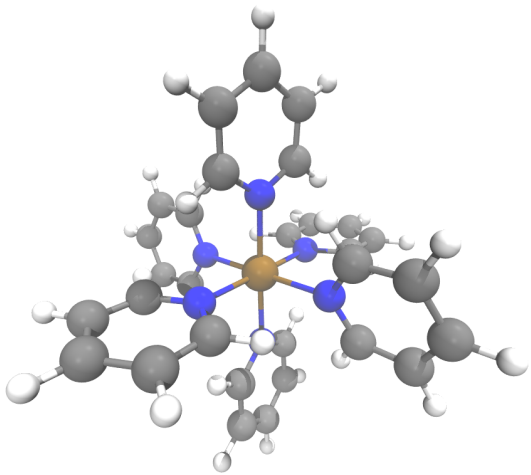

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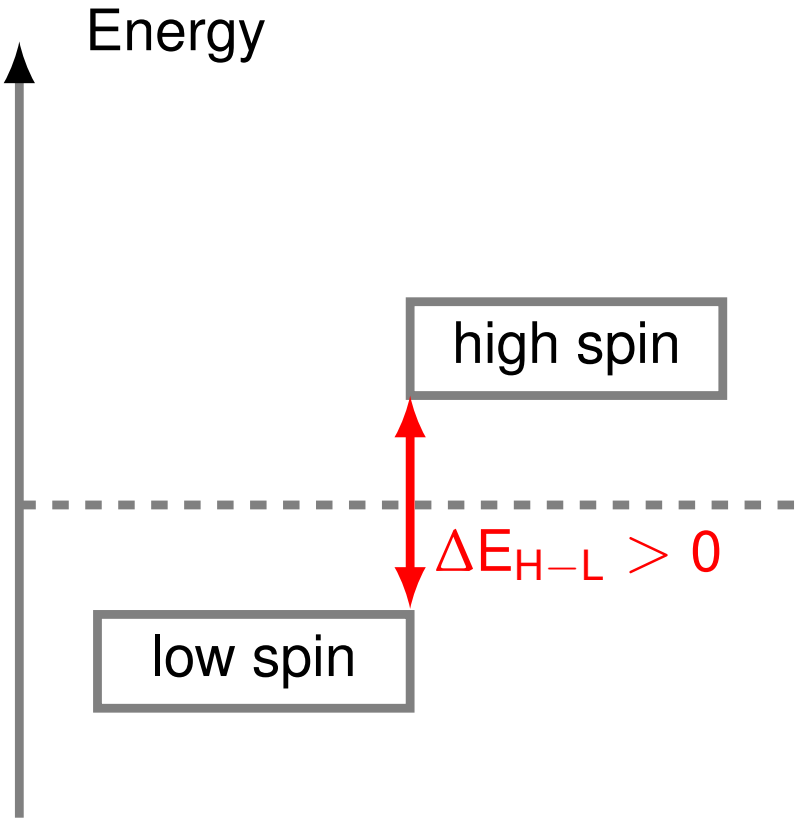

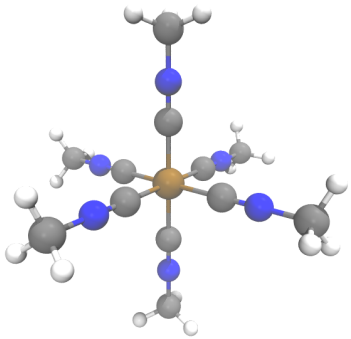

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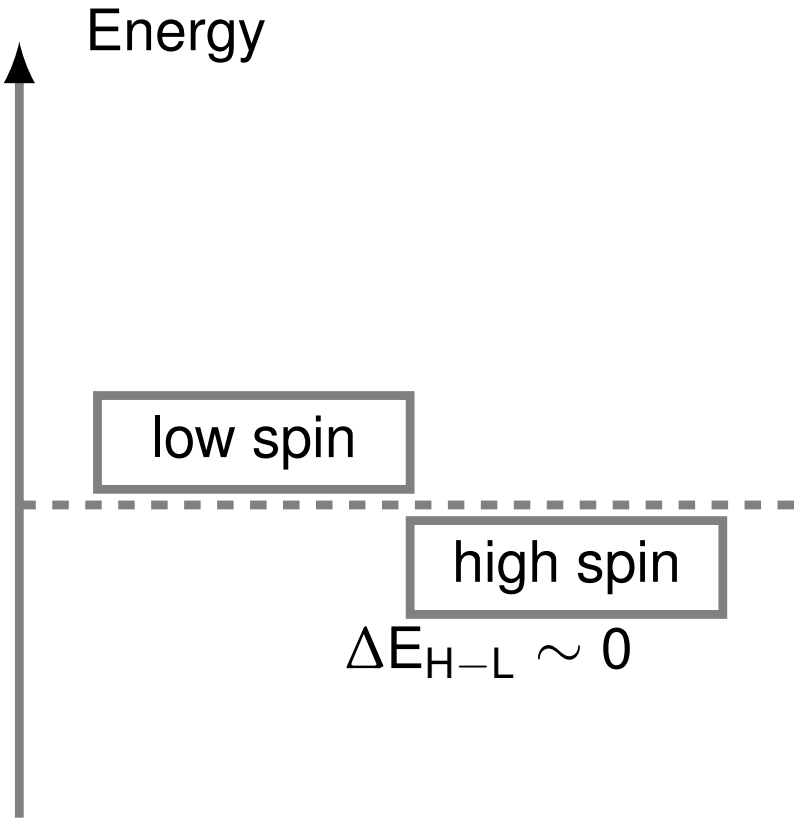

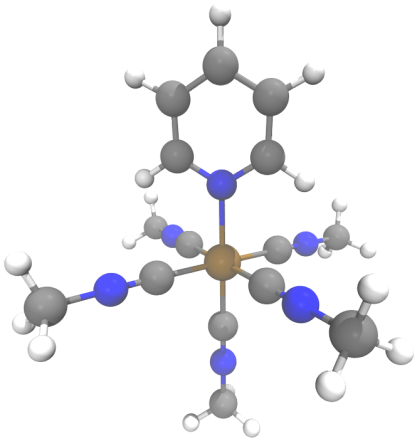

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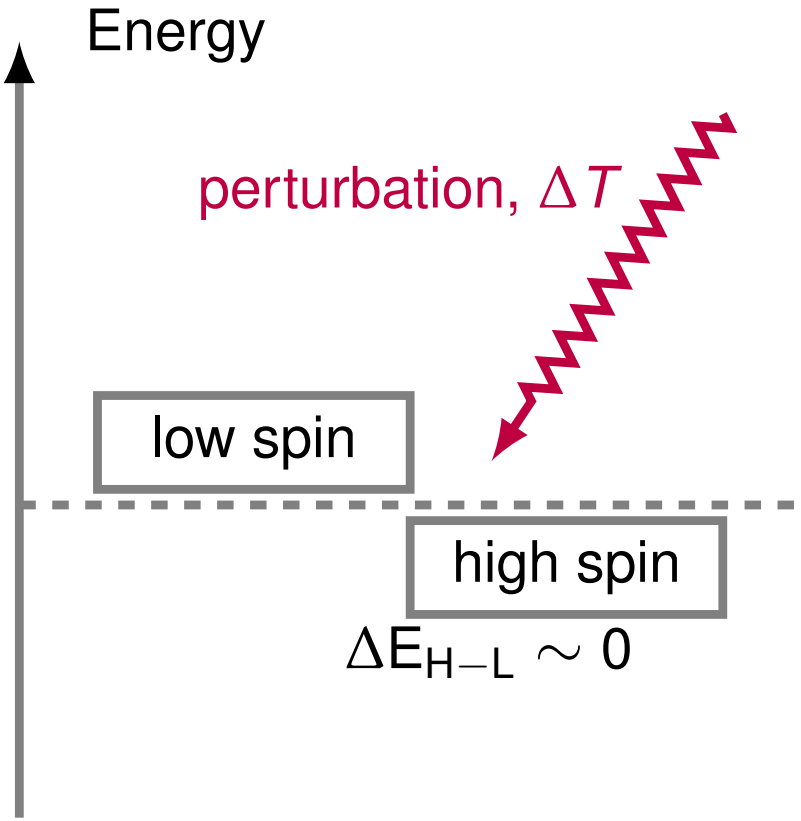

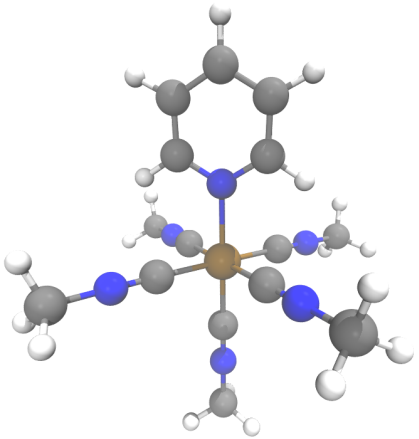

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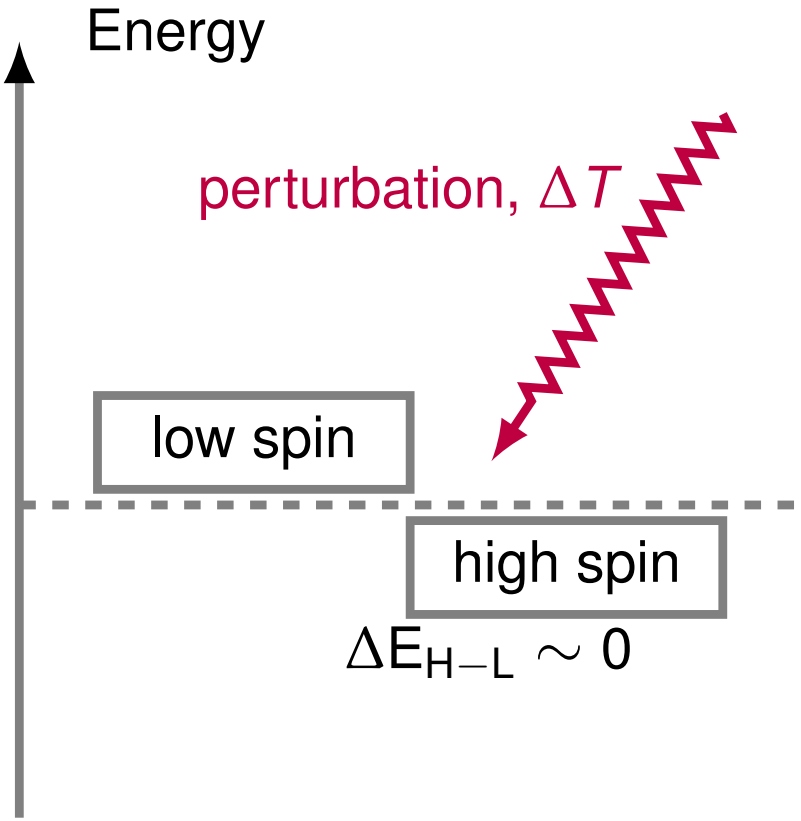

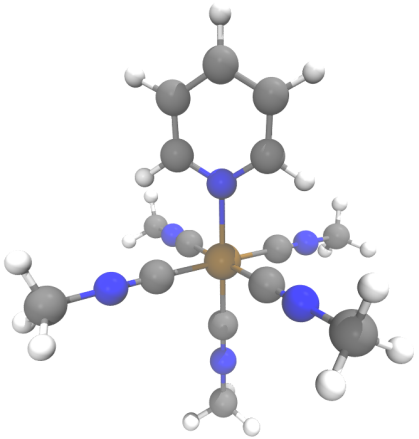

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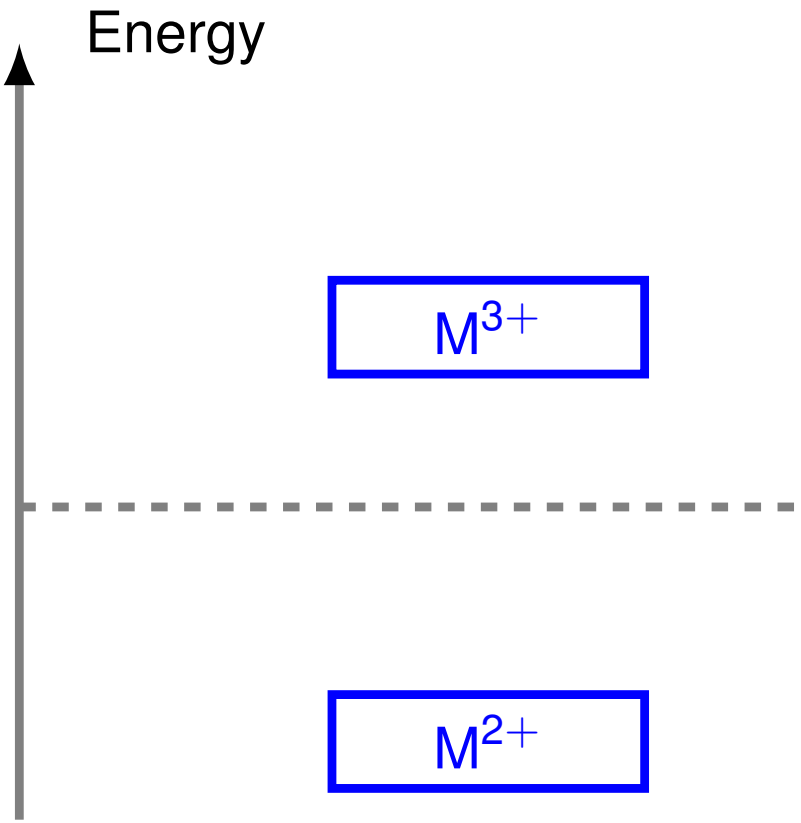

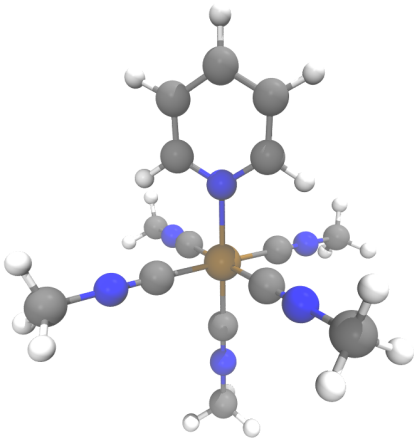

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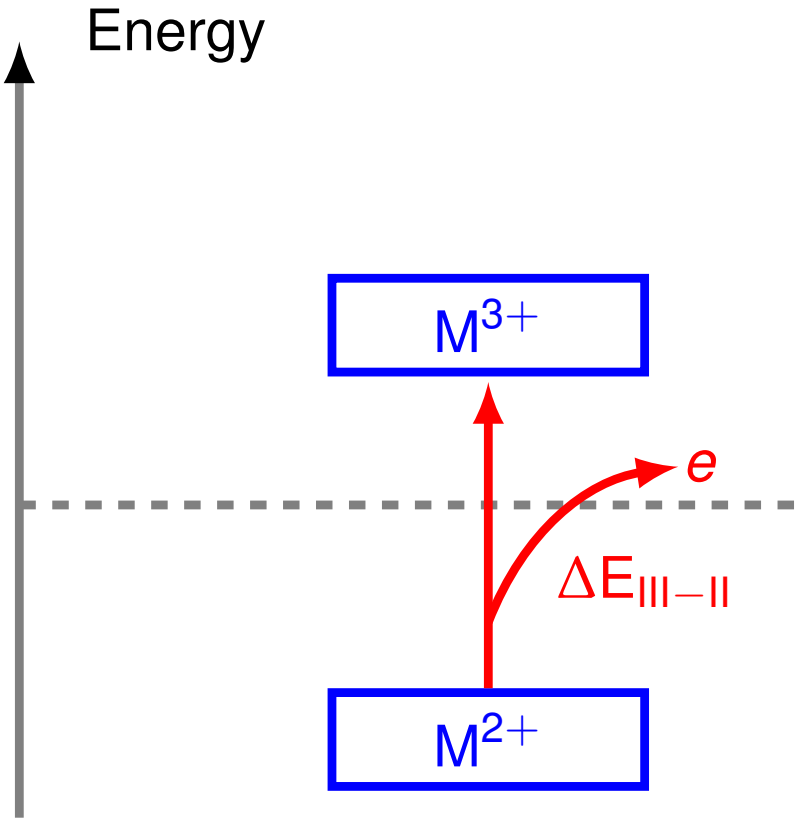

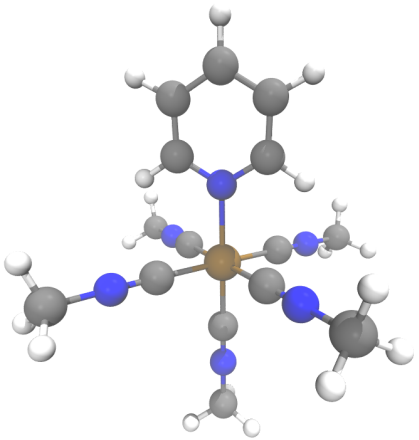

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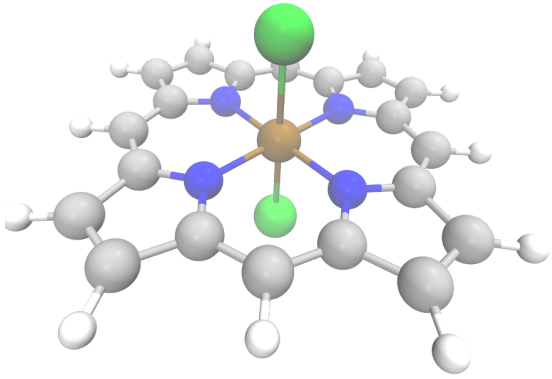

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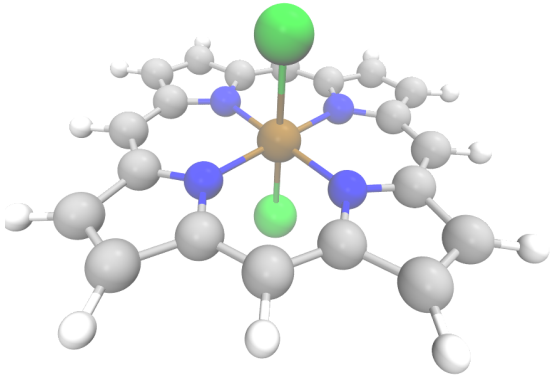

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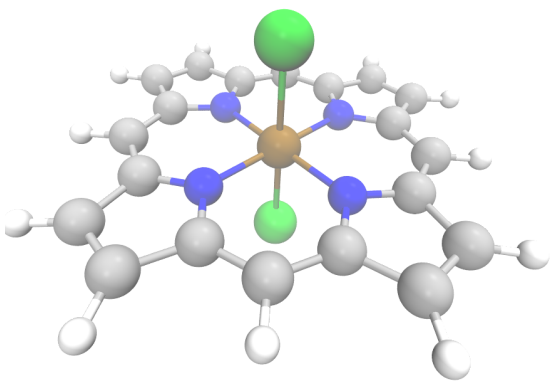

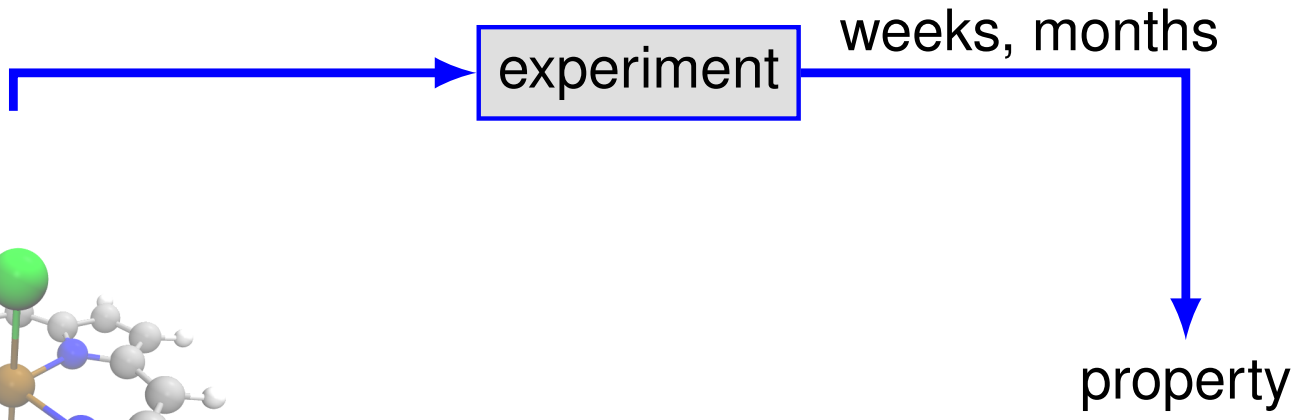

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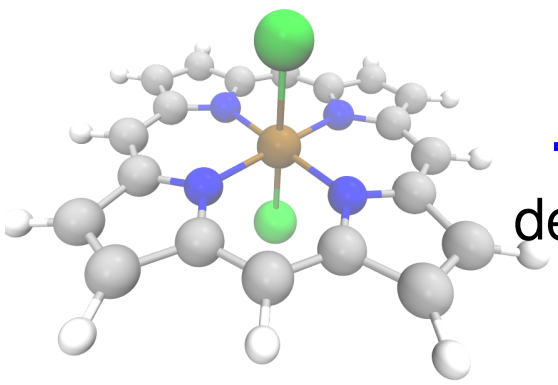

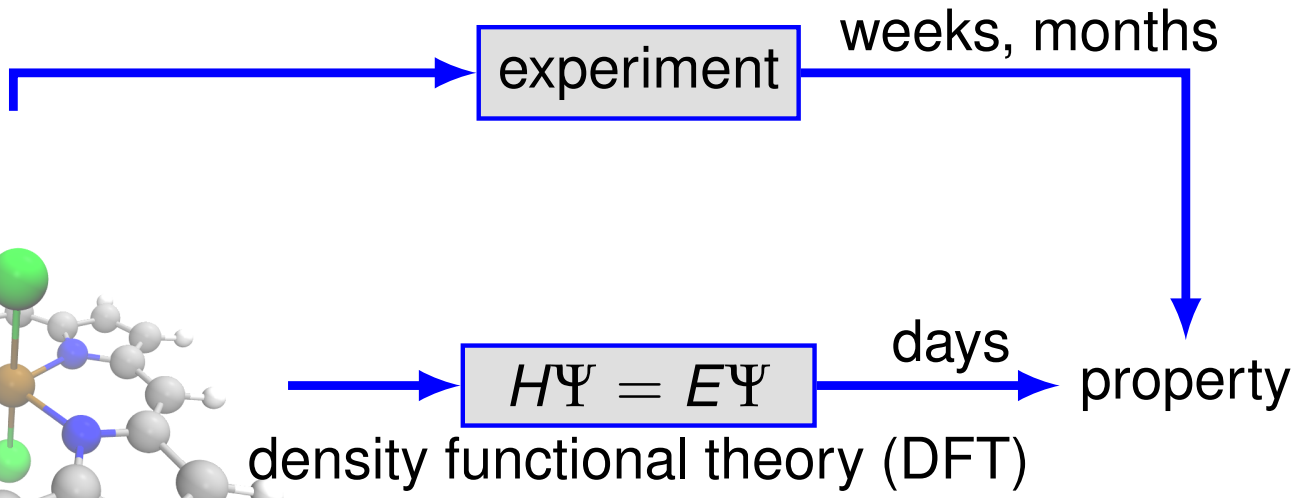

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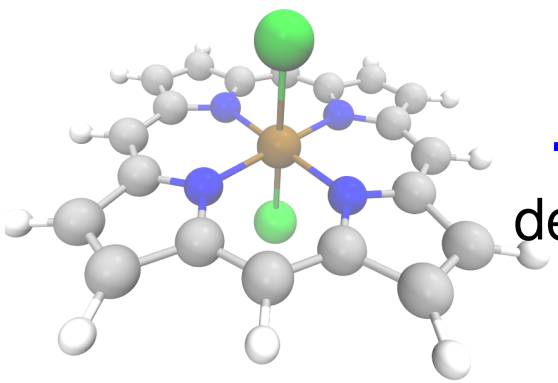

Input space design

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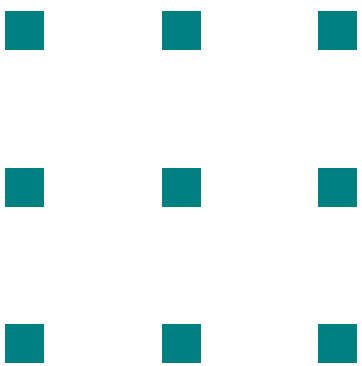

Chemical Space C_f

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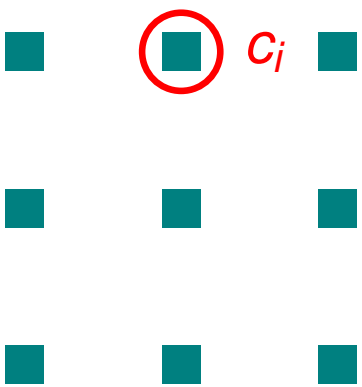

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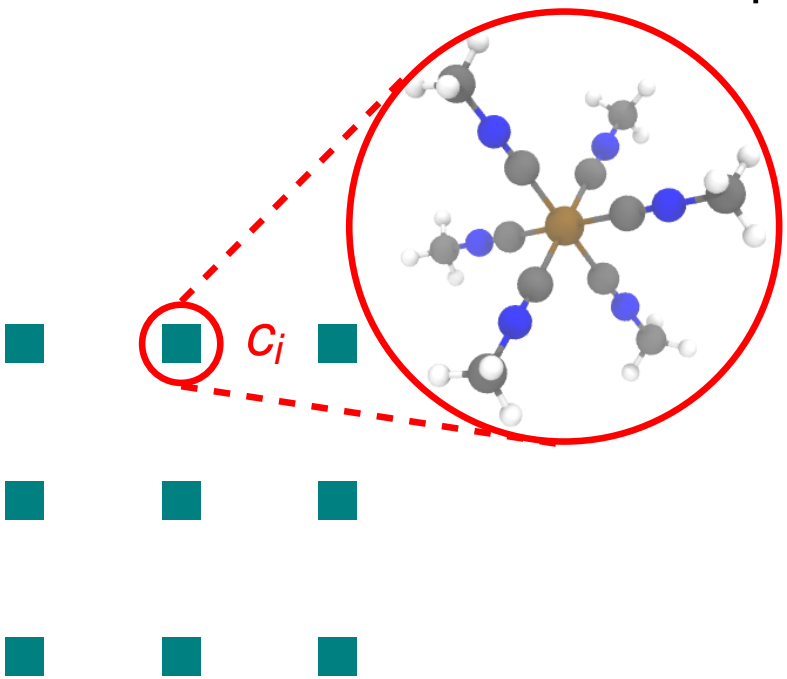

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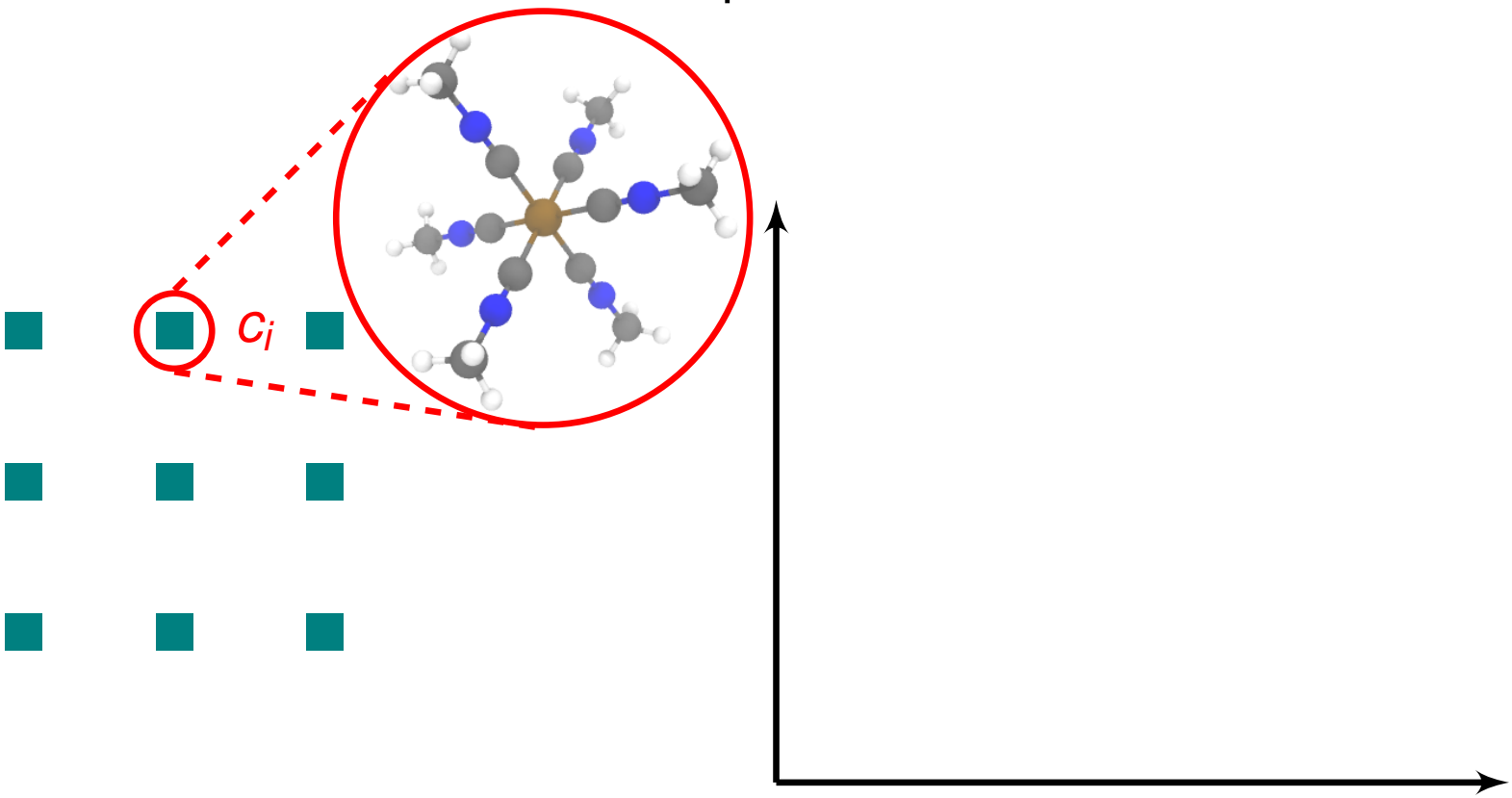
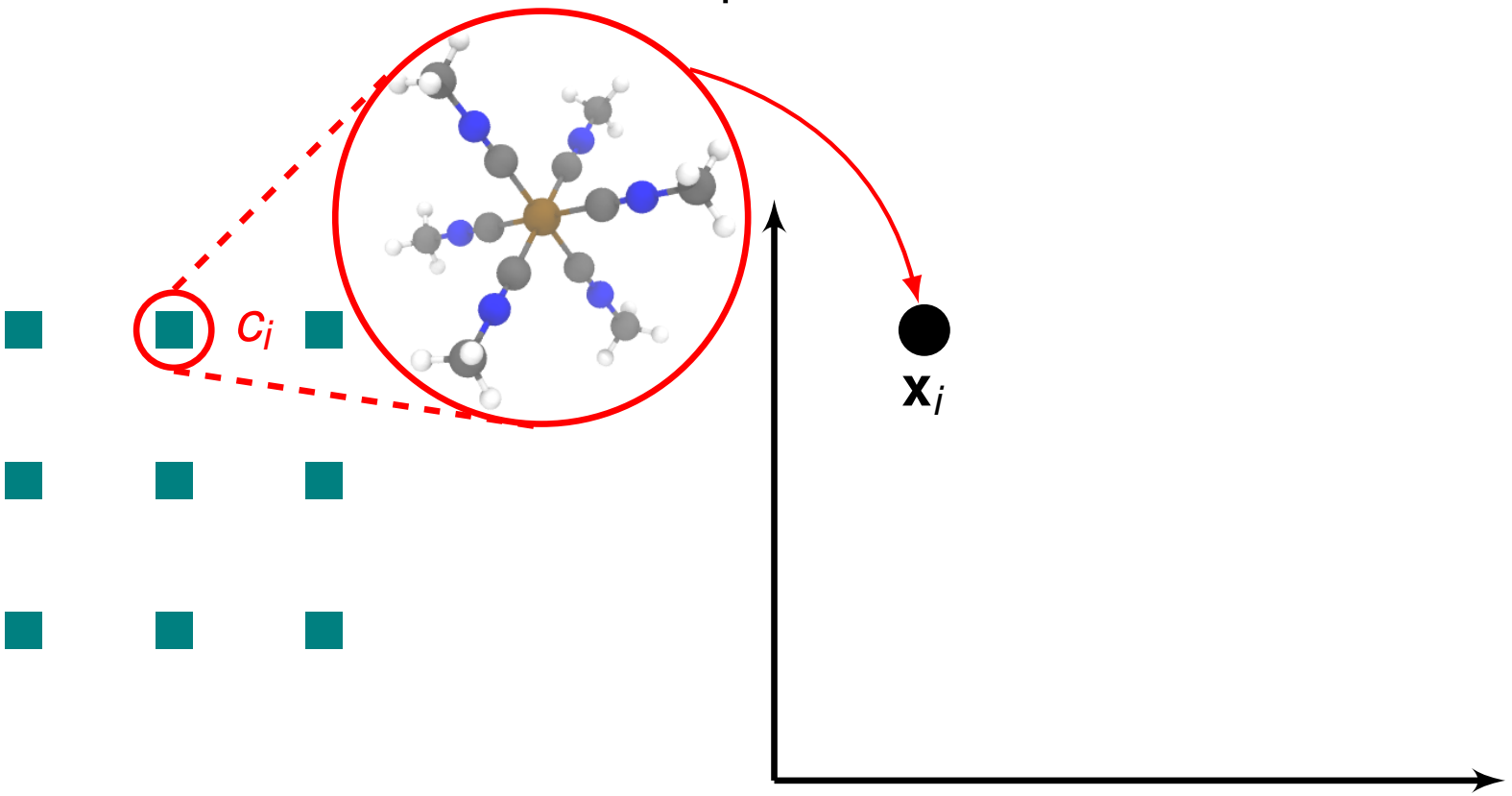


Chemical Space C_f

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

Input space design

What would be the ideal feature space?



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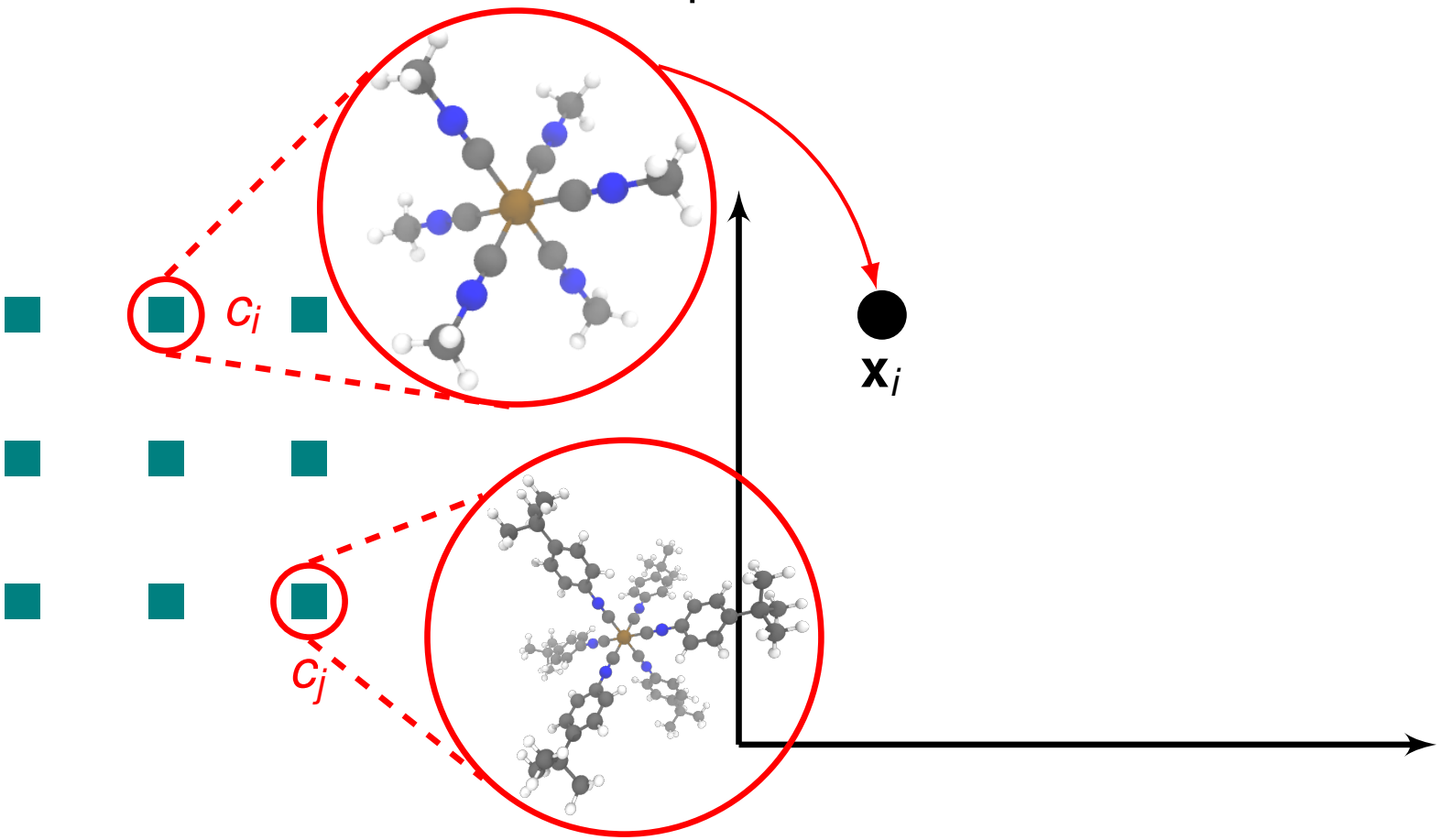

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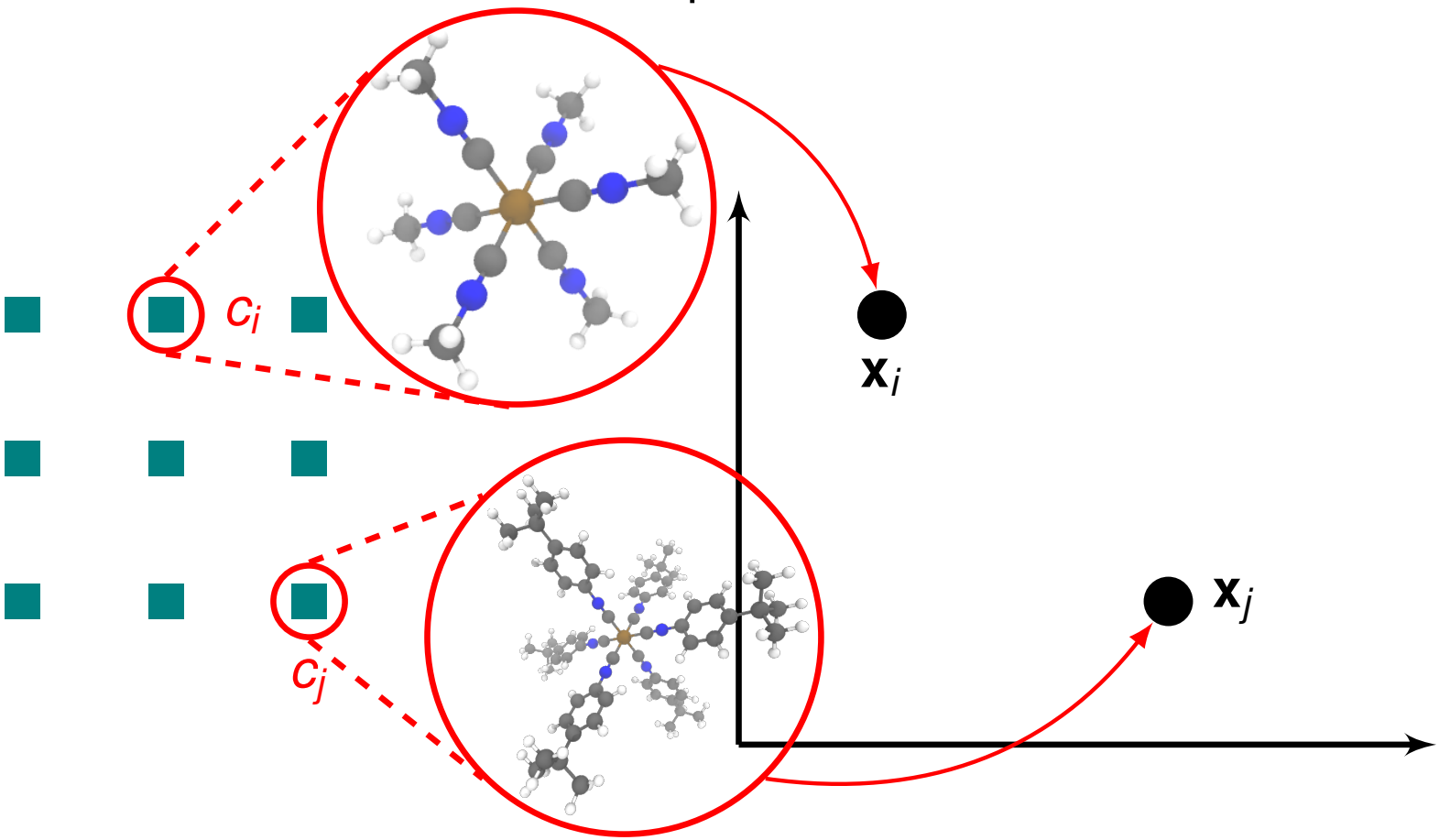

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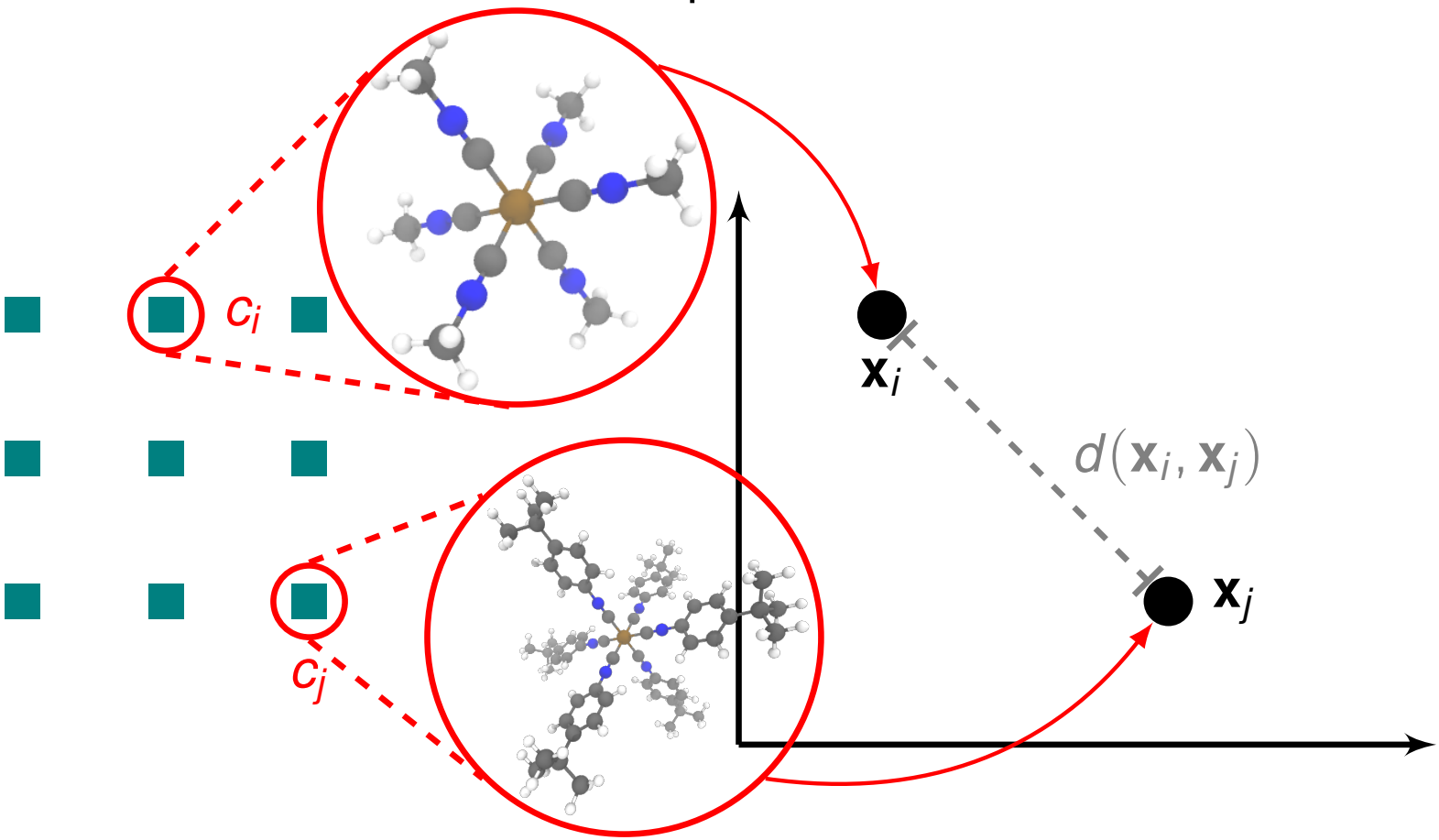

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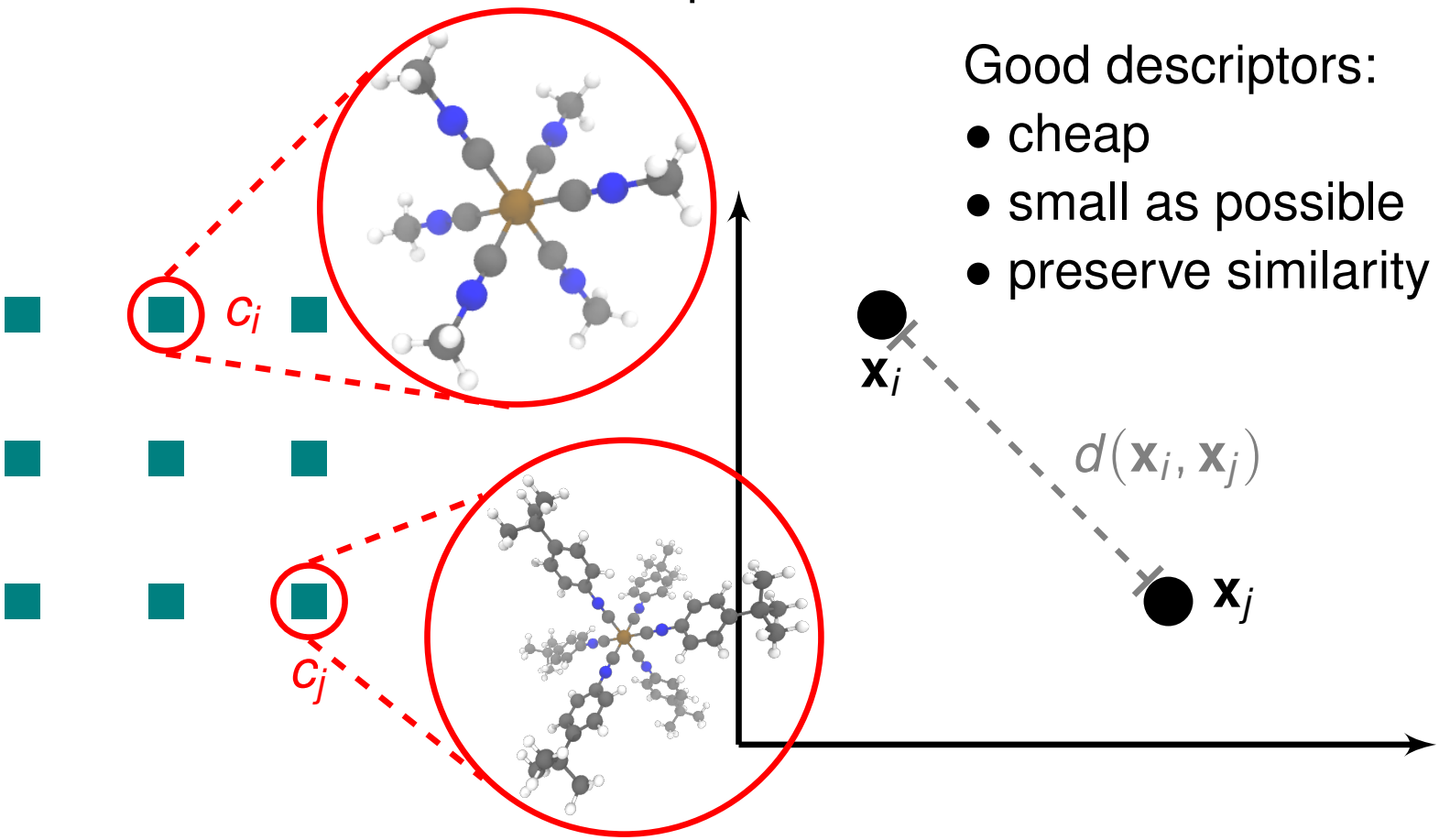


Good descriptors:

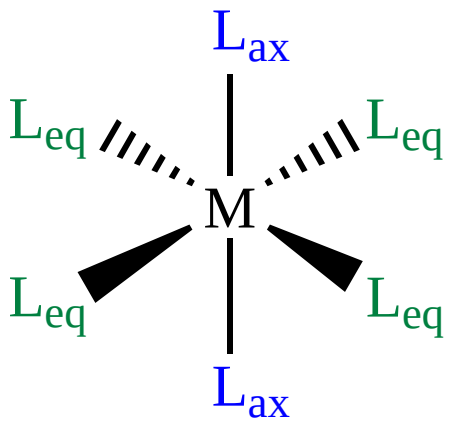
- cheap
- small as possible
- preserve similarity

Chemical Space C_f

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

Data for spin splitting

Data for octahedral complexes[1]:



[1] Janet, J.P., and Kulik, H.J. *Chem. Sci.*, 2017, 8, 5137-5152.

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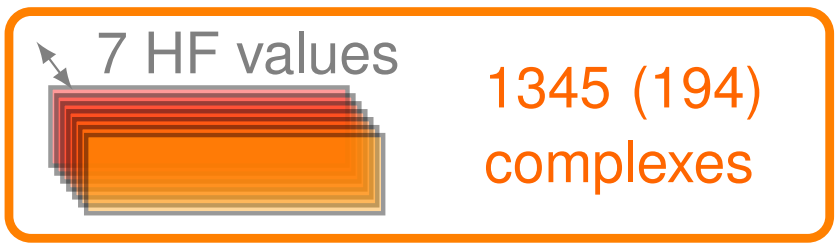

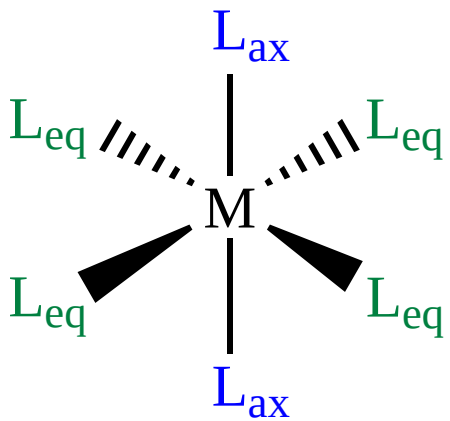

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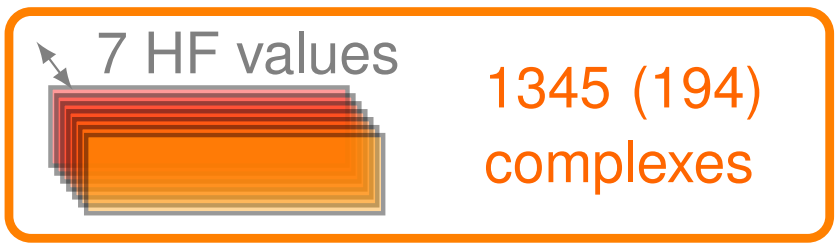

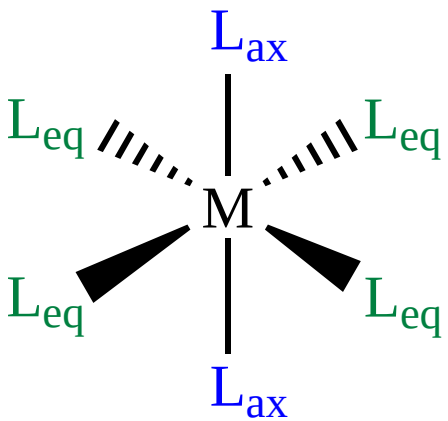

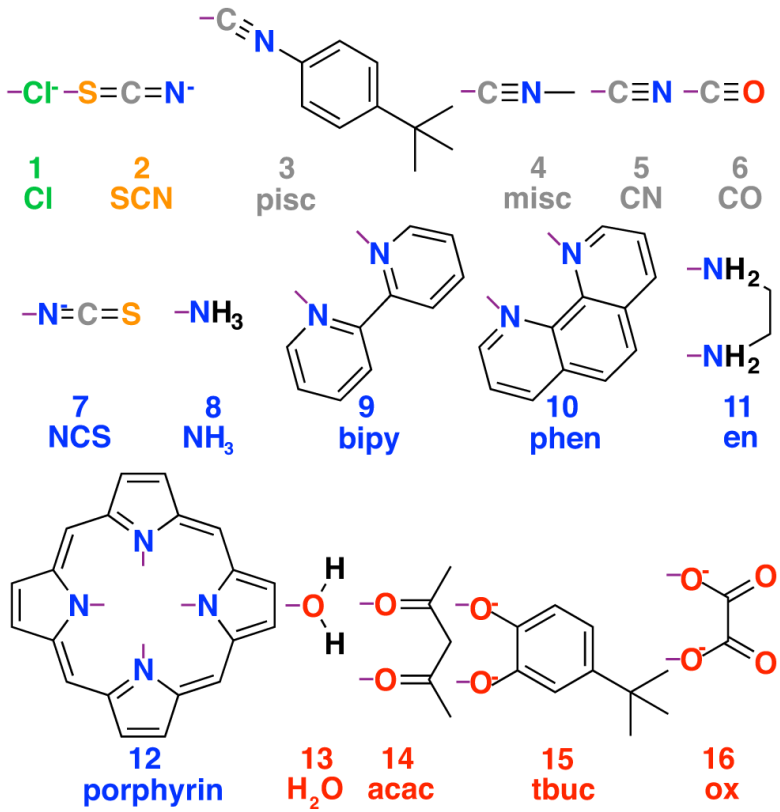

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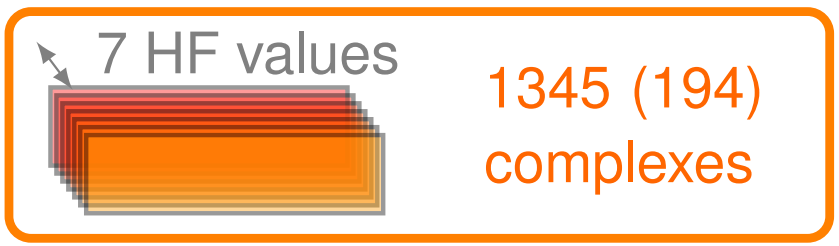

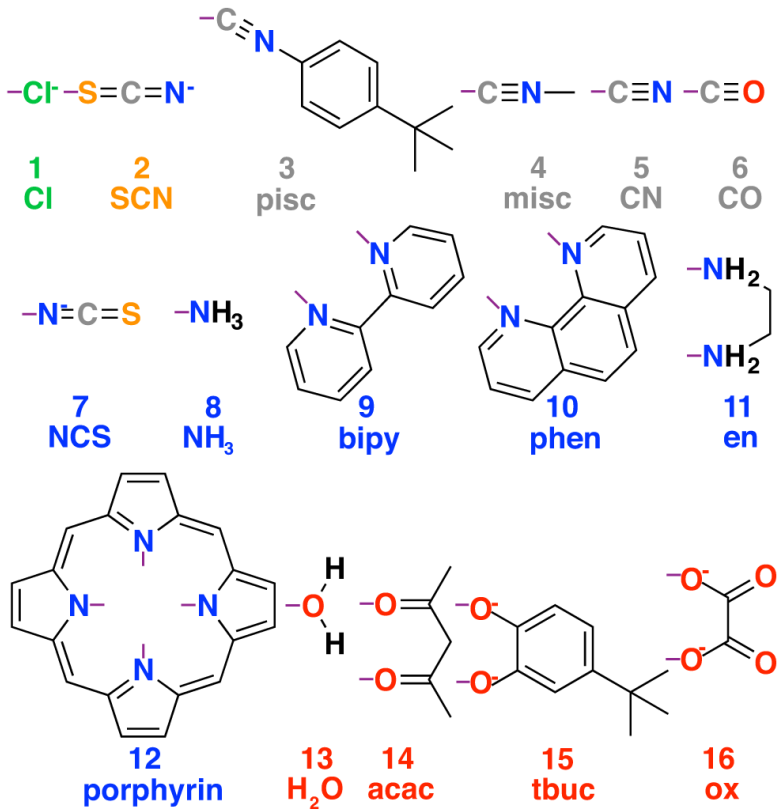

B3LYP-like DFT
HF exchange in 0-30%
gas phase optimizaton
LANL2DZ/6-31G*
high- and low-spin
M(II)/(III)

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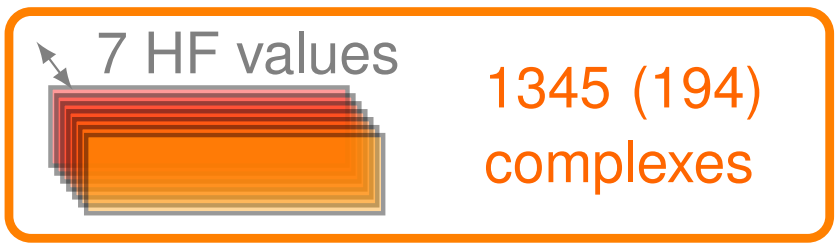

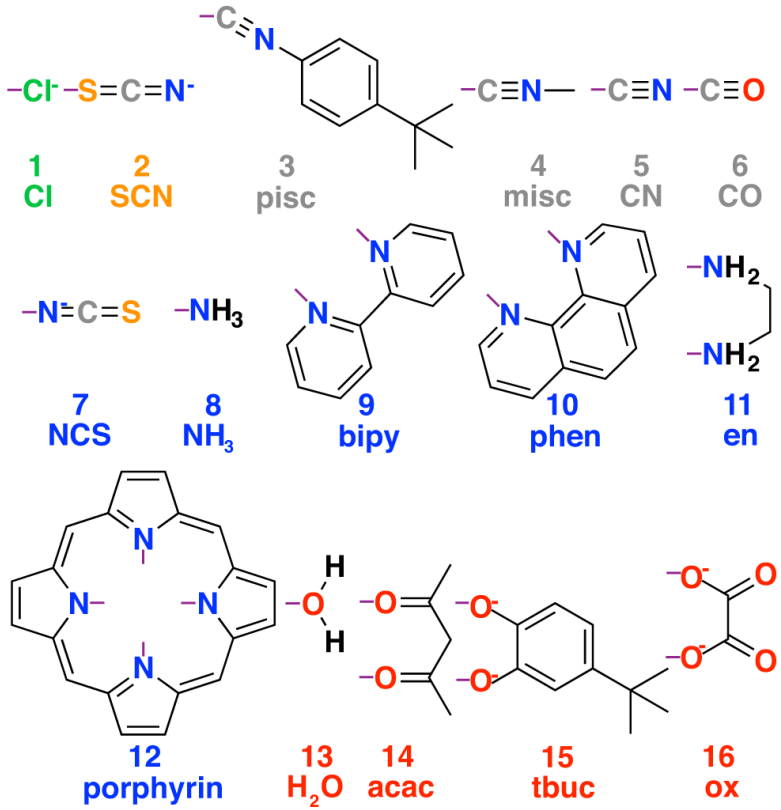

Coulomb matrix eigenspectrum (CM-ES) descriptor & kernel ridge regression (KRR)

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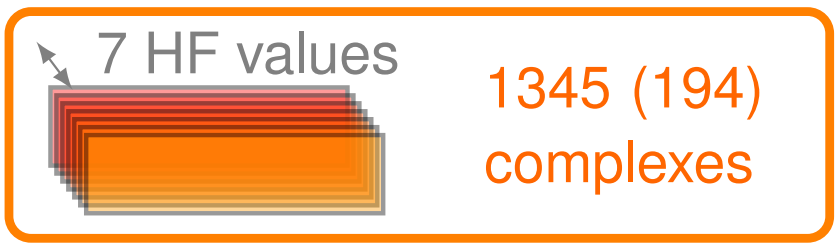

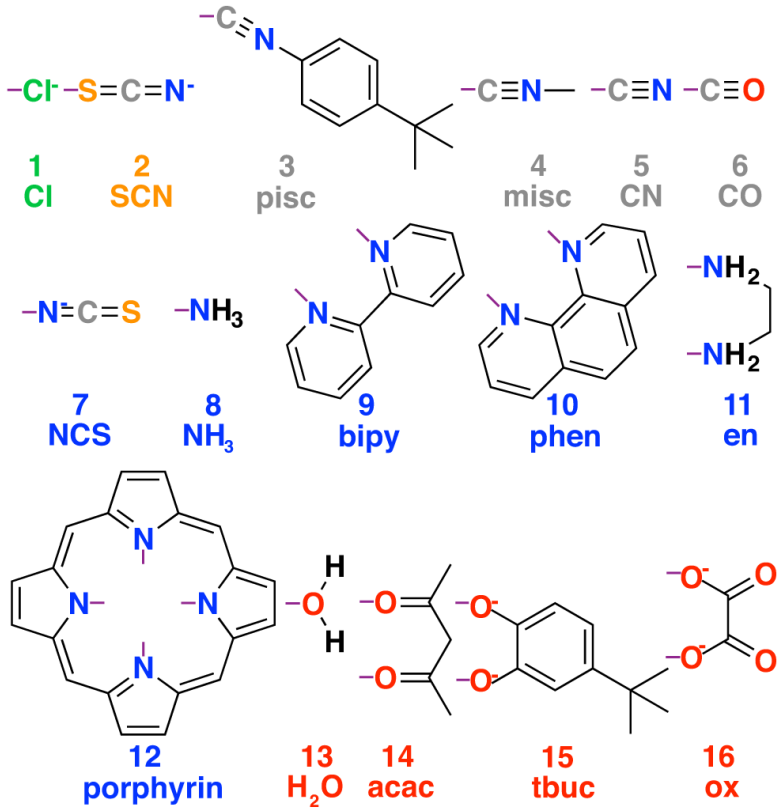

Coulomb matrix eigenspectrum (CM-ES) descriptor & kernel ridge regression (KRR)

	$\Delta E_{H\text{-}L}$ RMSE
CM-ES	19.2 kcal/mol

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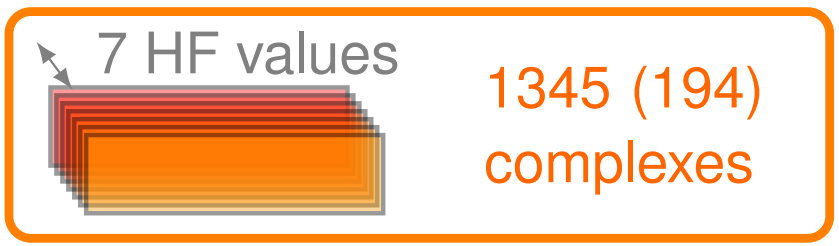

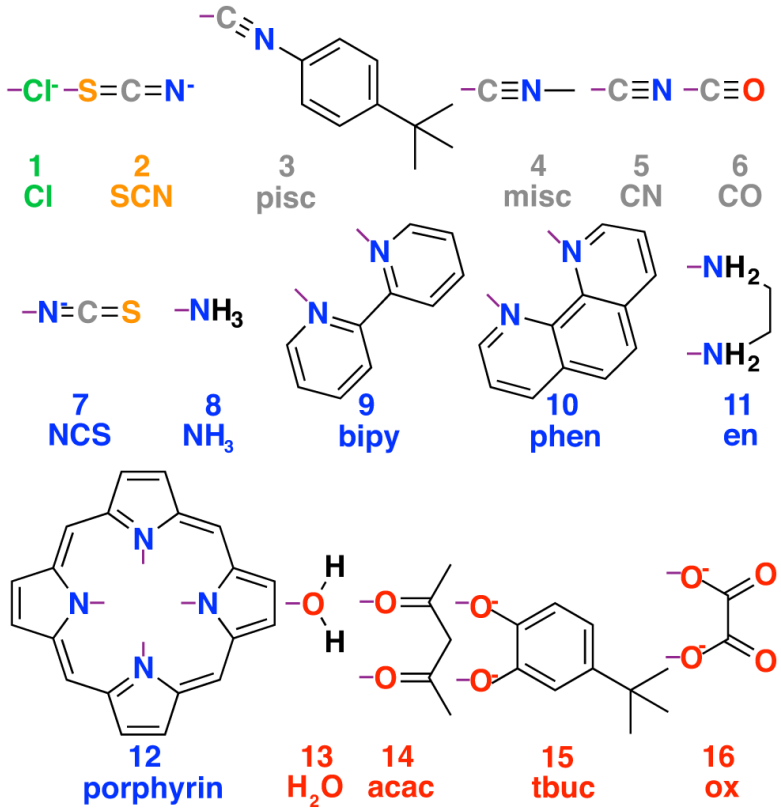

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Why?

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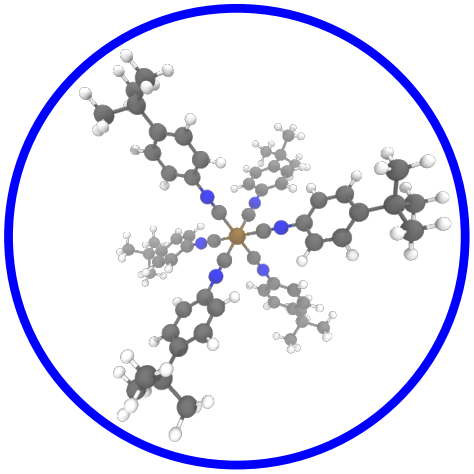
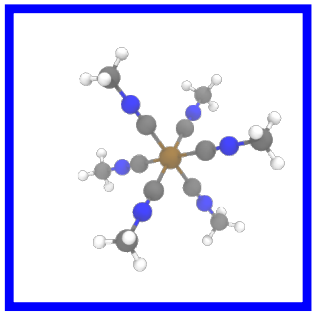
A tale of two complexes

$Fe[pisc]_6^{3+}$

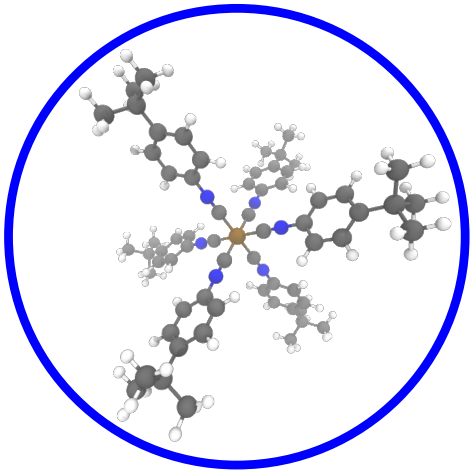


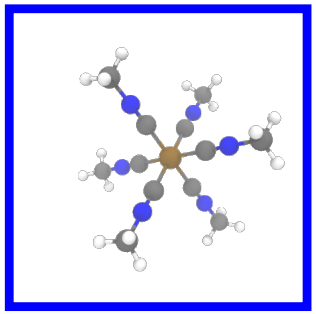


$Fe[misc]_6^{3+}$

A tale of two complexes

$Fe[pisc]_6^{3+}$



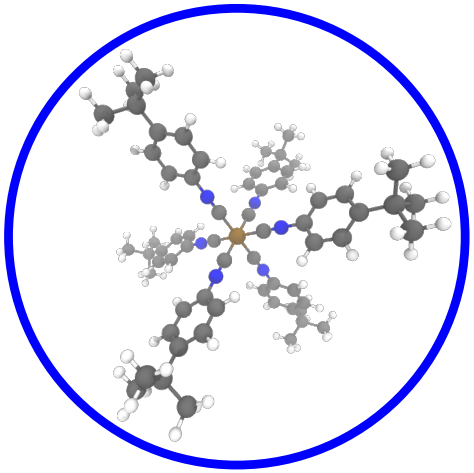


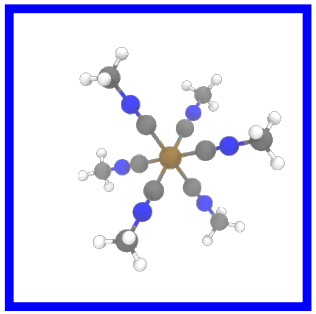
$Fe[misc]_6^{3+}$

$\Delta E_{H\text{-}L} = 37.7$ kcal/mol $\Delta E_{H\text{-}L} = 40.7$ kcal/mol

A tale of two complexes

$Fe[pisc]_6^{3+}$





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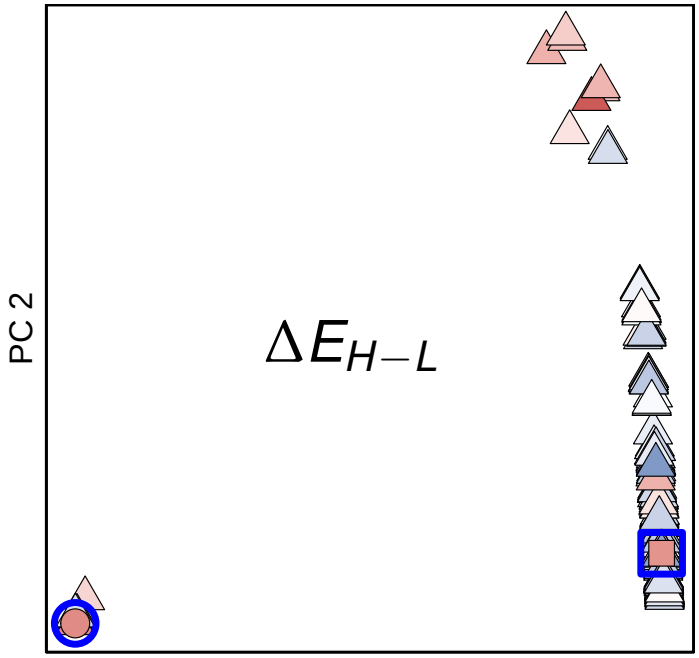

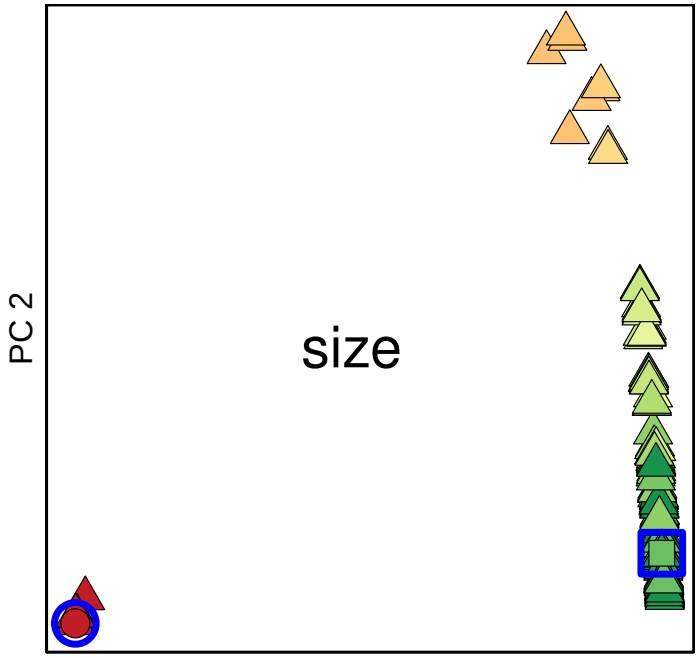

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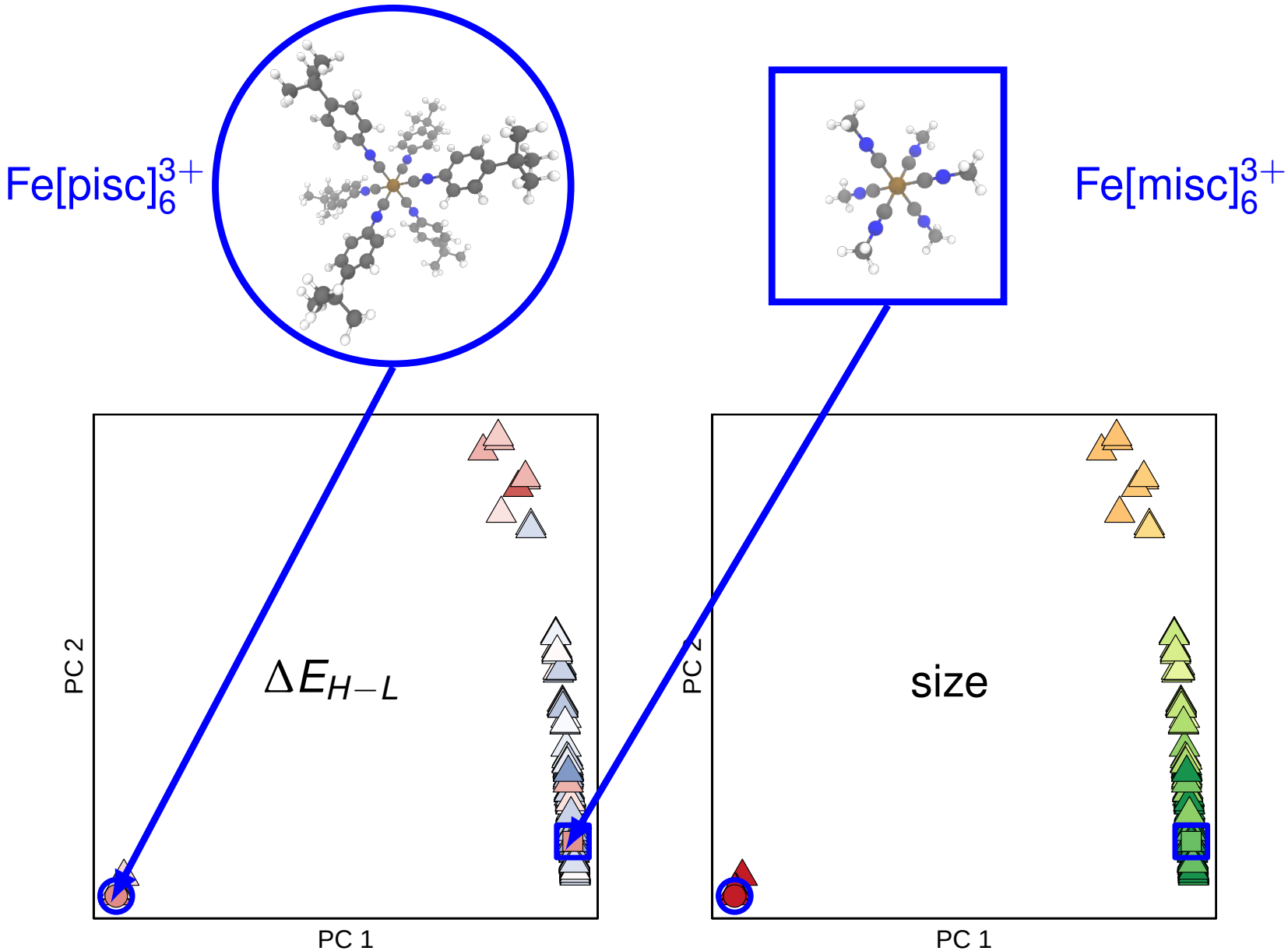

MCDL-25

mixed continuous discrete lcoal (MCDL)

MCDL-25

mixed continuous discrete lcoal (MCDL)

metal

properties

identity

Fe(II)

oxidation state

Janet, J.P., and Kulik, H.J. *Chem. Sci.*, 2017, 8, 5137-5152.

MCDL-25

mixed continuous discrete lcoal (MCDL)

metal properties

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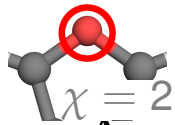
oxidation state

local ligand properties

$\chi = 3.44$



$\chi = 2.55$

max $\Delta\chi$

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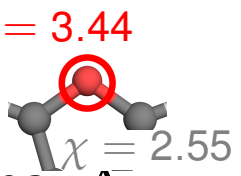
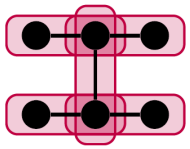
MCDL-25

mixed continuous discrete lcoal (MCDL)

metal properties	local ligand properties	global ligand properties
identity	$\chi = 3.44$	
Fe(II)	$\chi = 2.55$	
oxidation state	max $\Delta\chi$	Kier index





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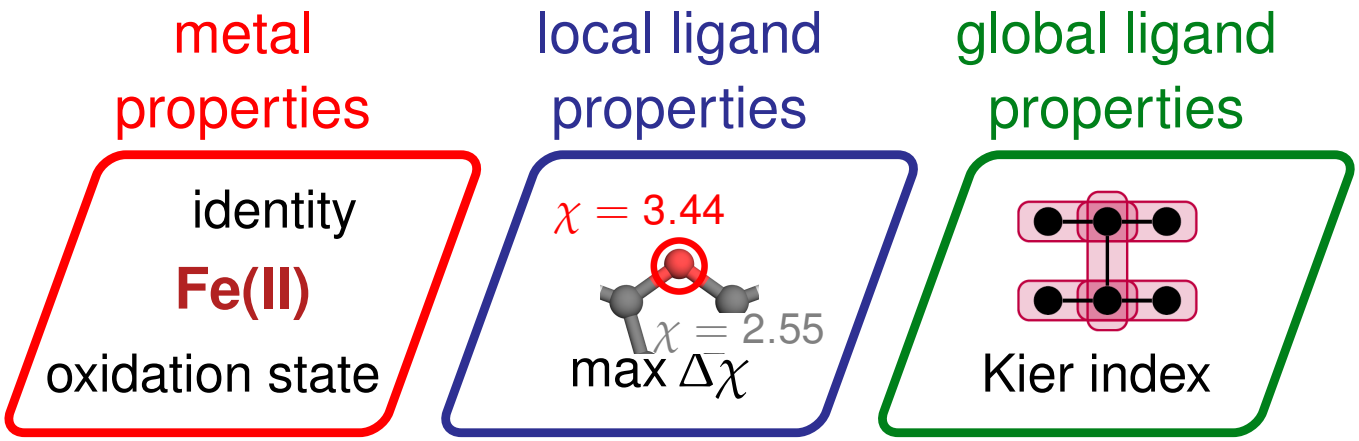

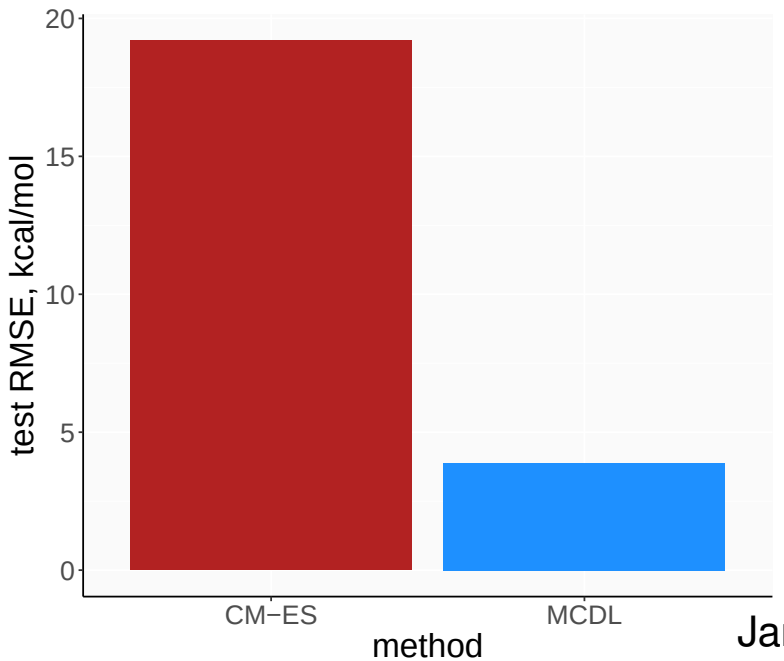

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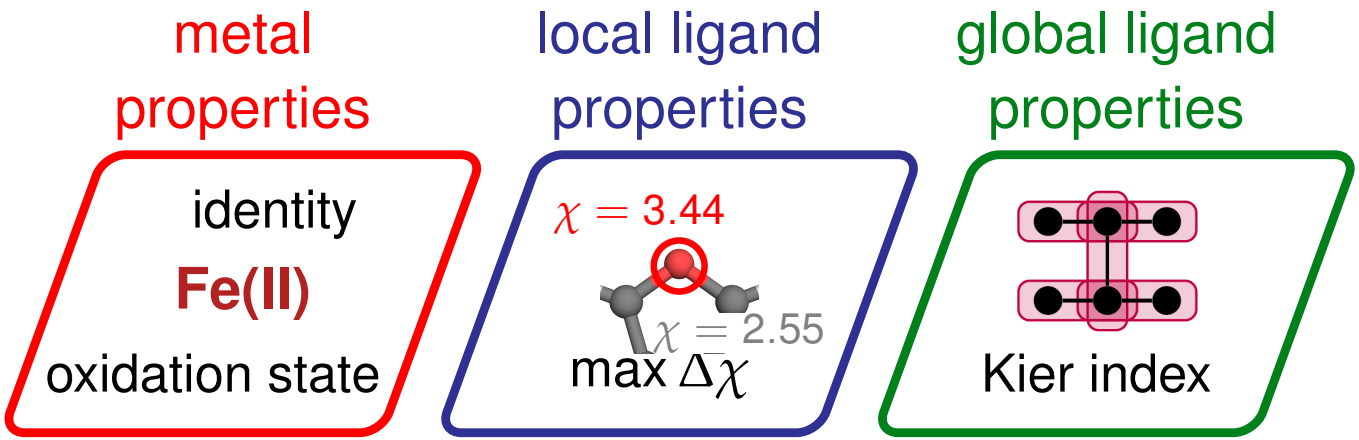

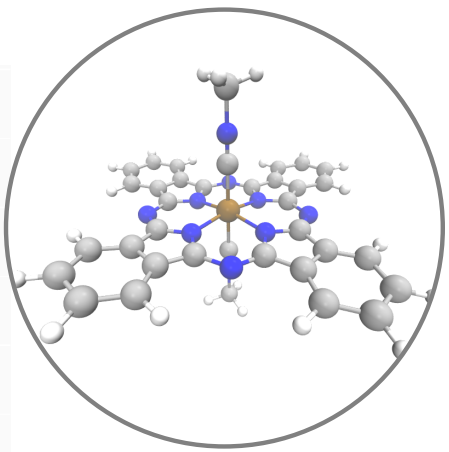

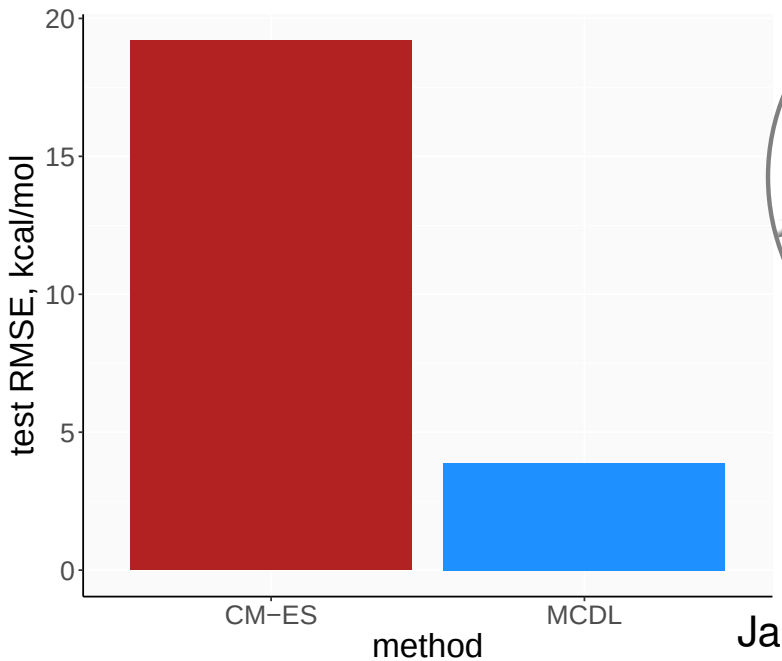

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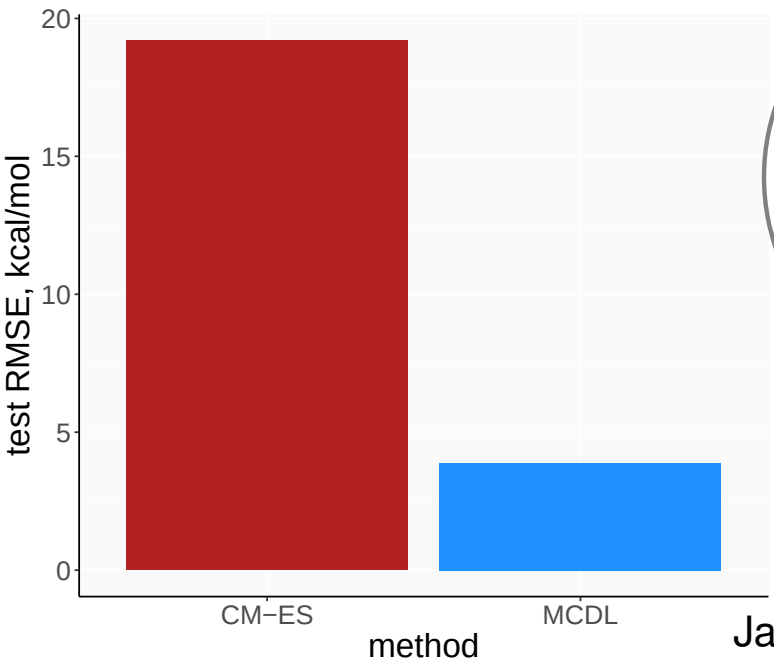

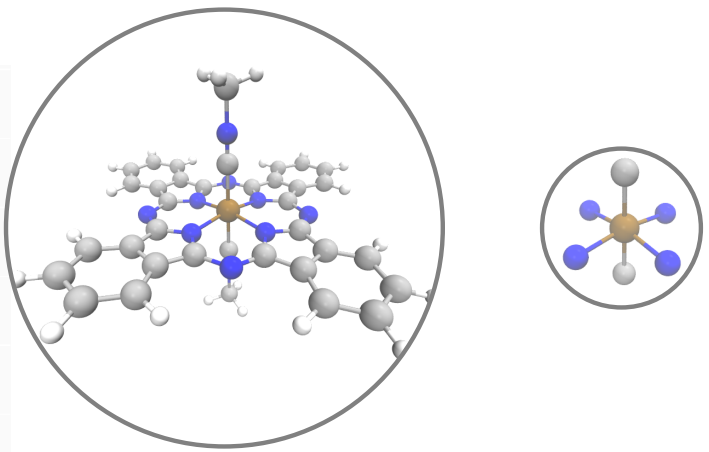

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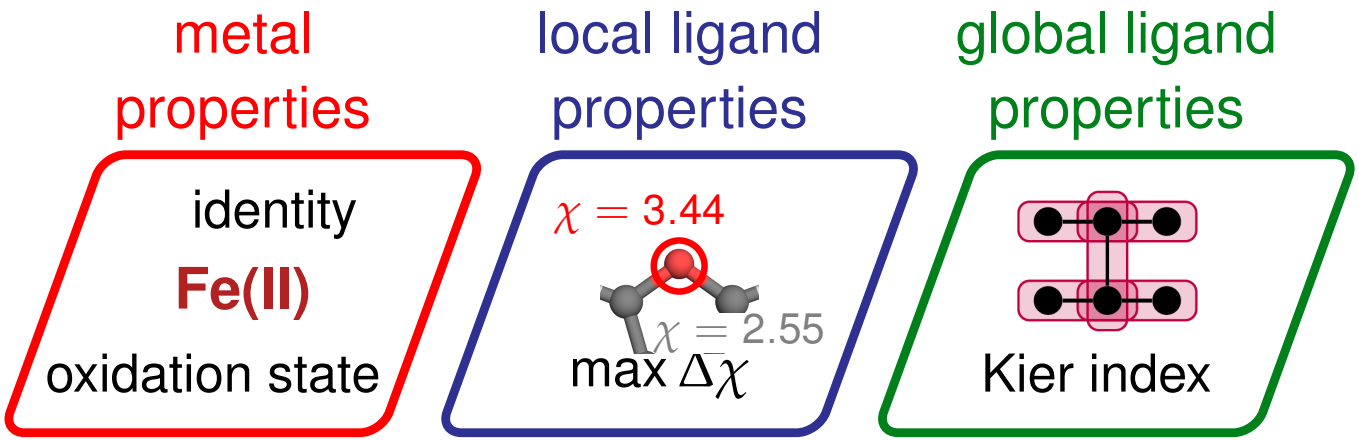
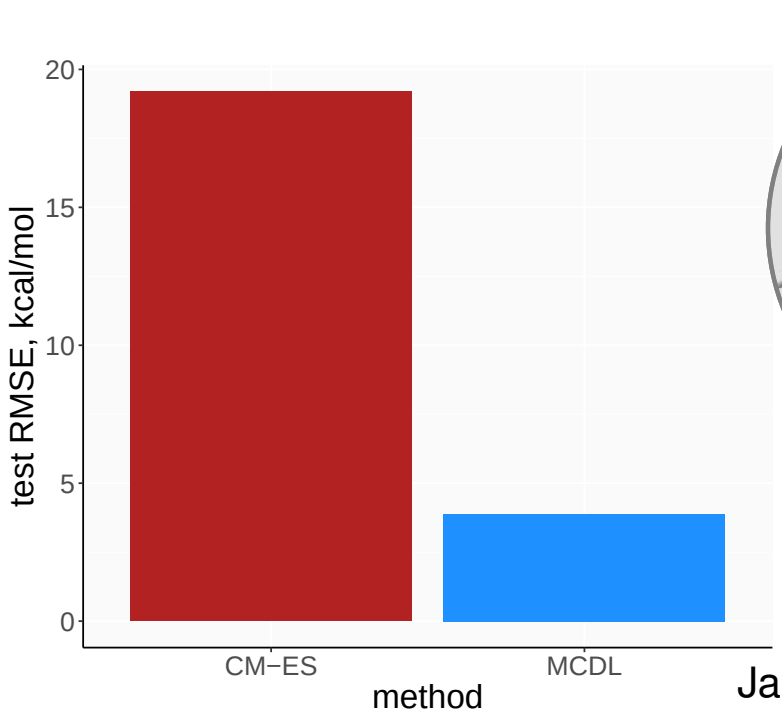
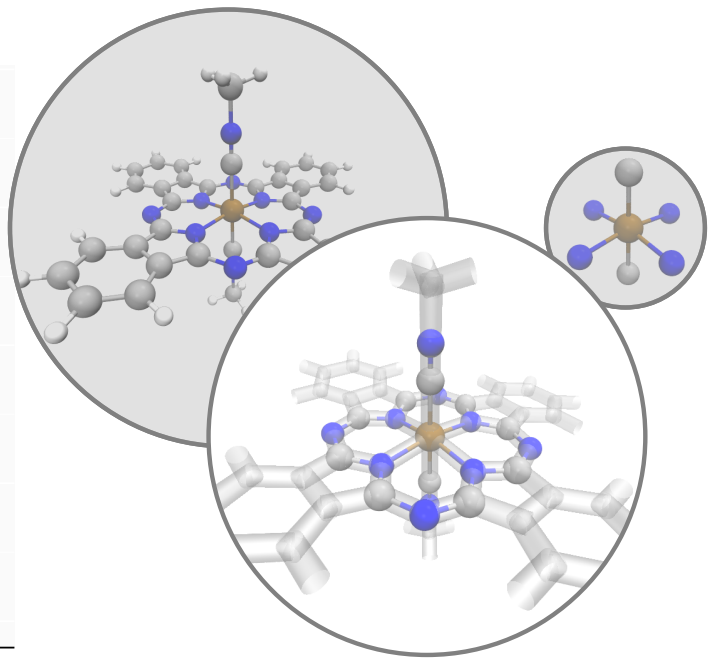


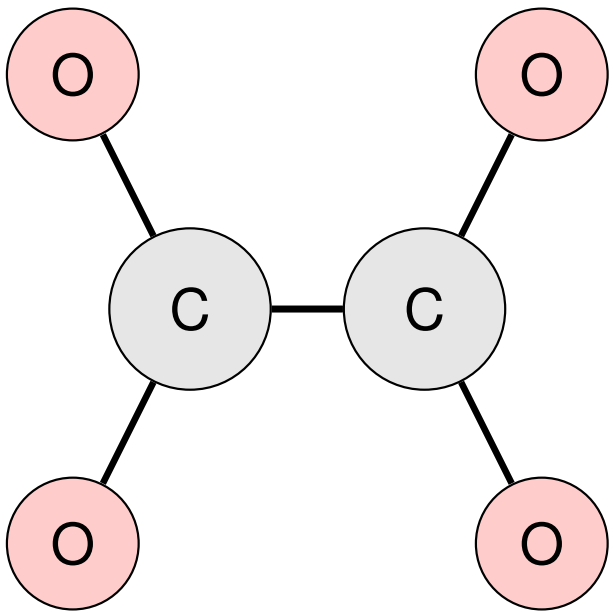




Janet, J.P., and Kulik, H.J. *Chem. Sci.*, 2017, 8, 5137-5152.

Extensible, continuous descriptors - RACs

Based on autocorrelations[2]



[2]Broto, P., Moreau, G. and Vandycke, C. *Eur. J. Med. Chem.*, 19(1):71-78, 1984.

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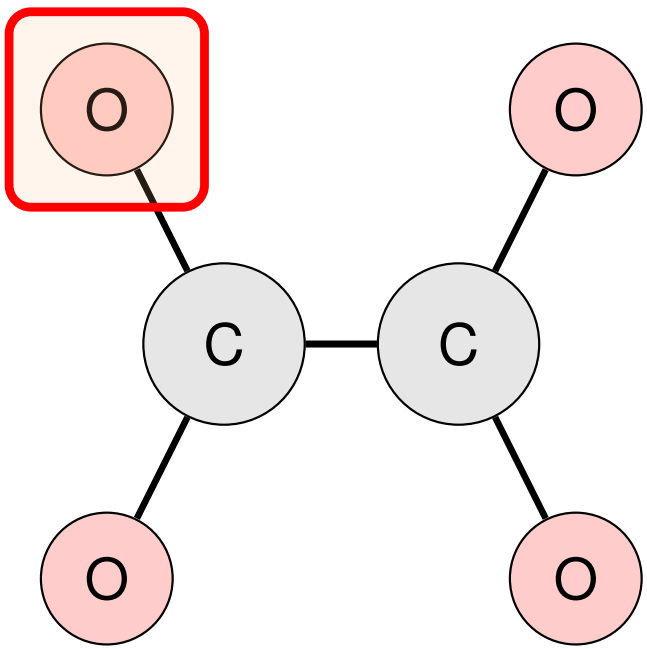

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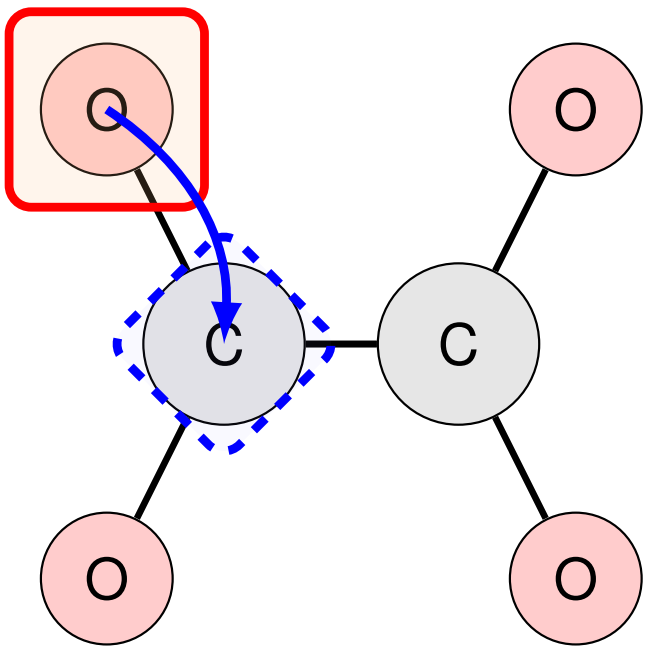
Extensible, continuous descriptors - RACs

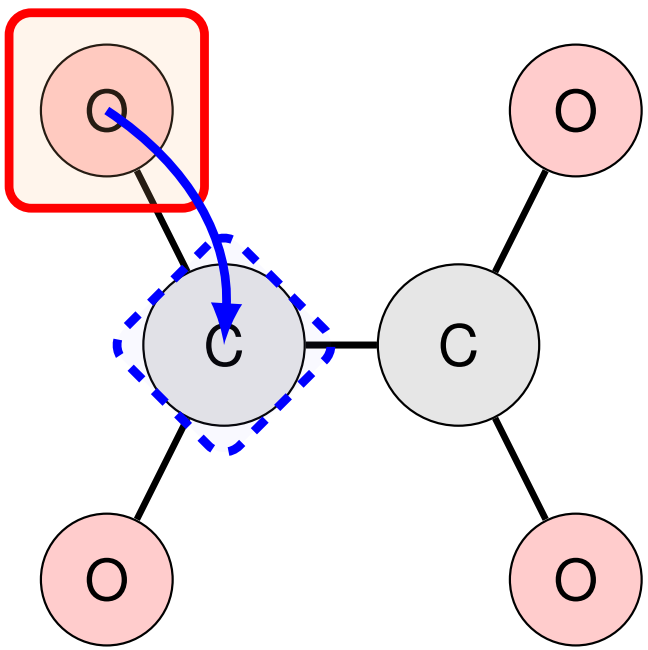
Based on autocorrelations[2]



[2]Broto, P., Moreau, G. and Vandycke, C. *Eur. J. Med. Chem.*, 19(1):71-78, 1984.

Extensible, continuous descriptors - RACs

Based on autocorrelations[2]

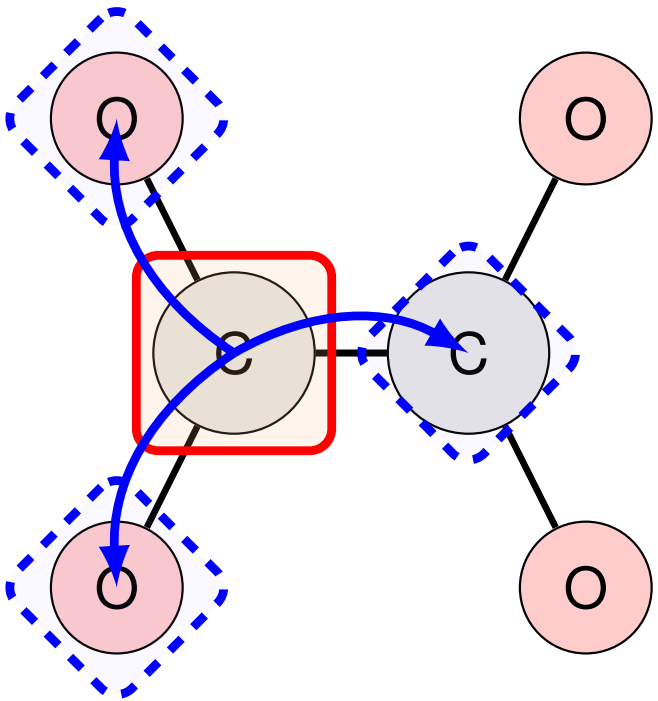


$$d_1 : \sum_{O,C} Z_O Z_C = 48$$

[2]Broto, P., Moreau, G. and Vandycke, C. *Eur. J. Med. Chem.*, 19(1):71-78, 1984.

Extensible, continuous descriptors - RACs

Based on autocorrelations[2]

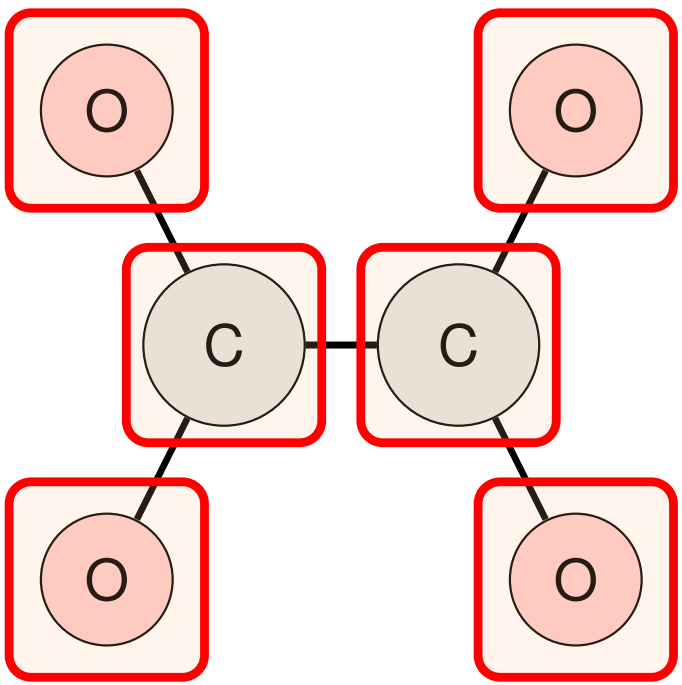


$$d_1 : 48 + \sum_{C,O} Z_O Z_C = 144 + 48$$

[2]Broto, P., Moreau, G. and Vandycke, C. *Eur. J. Med. Chem.*, 19(1):71-78, 1984.

Extensible, continuous descriptors - RACs

Based on autocorrelations[2]

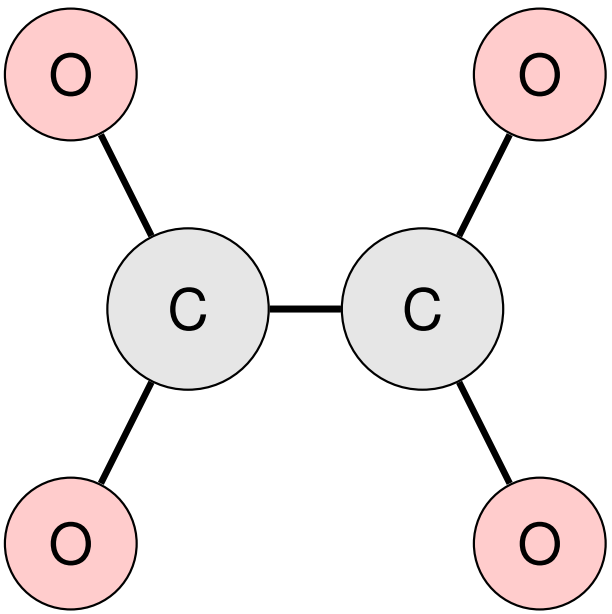


$$d_1 : \sum_i \sum_j Z_i Z_j \delta(d_{i,j}, 1)$$

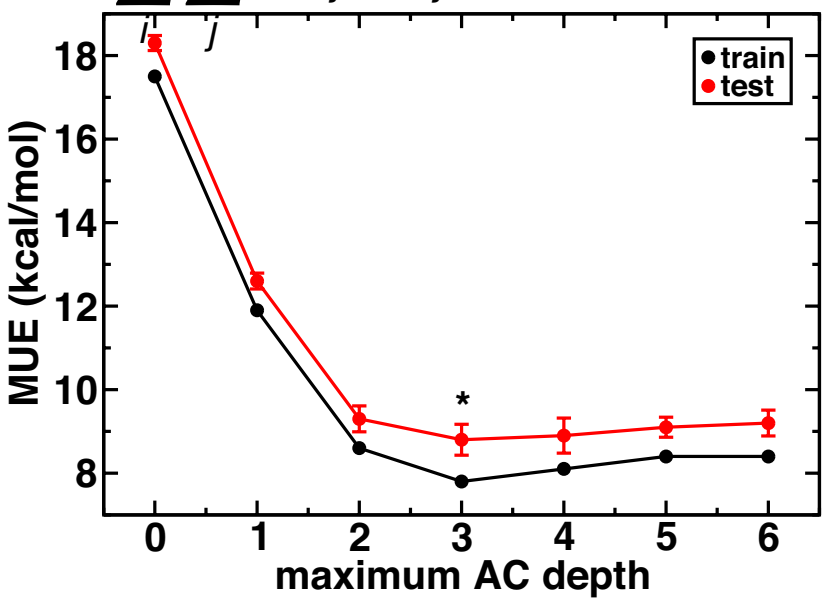
[2]Broto, P., Moreau, G. and Vandycke, C. *Eur. J. Med. Chem.*, 19(1):71-78, 1984.

Extensible, continuous descriptors - RACs

Based on autocorrelations[2]



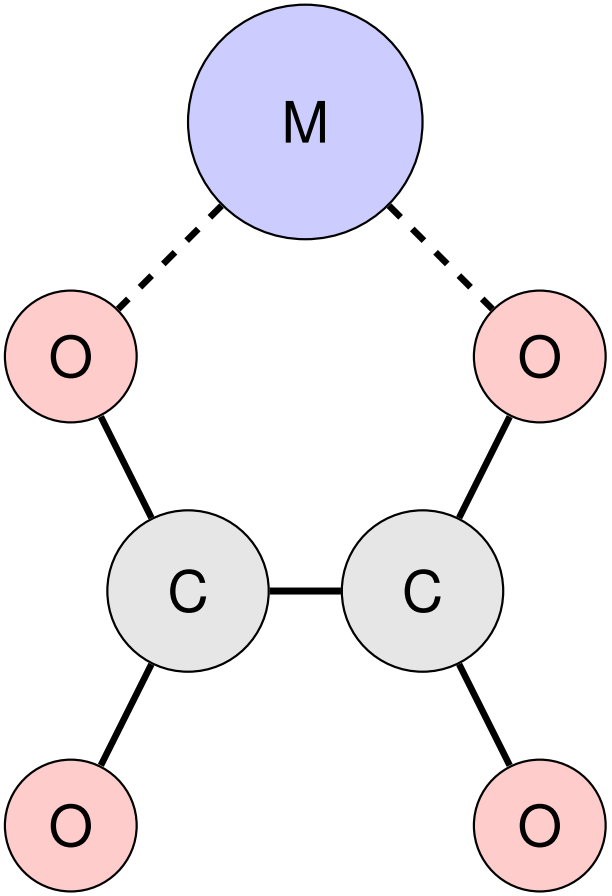
$$d_x : \sum_i \sum_j Z_i Z_j \delta(d_{ij}, x)$$



[2]Broto, P., Moreau, G. and Vandycke, C. *Eur. J. Med. Chem.*, 19(1):71-78, 1984.

Extensible, continuous descriptors - RACs

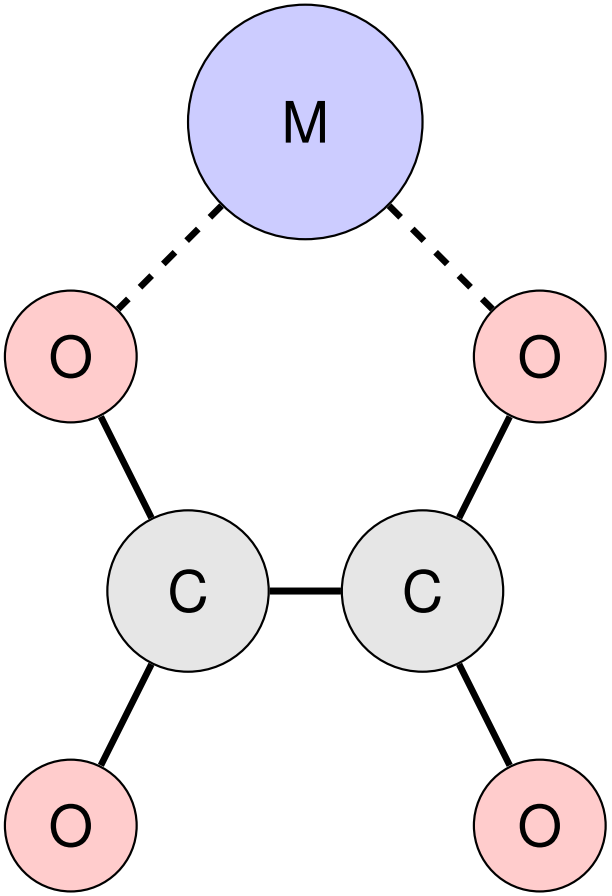
Based on autocorrelations



How to adapt to TM complexes?

Extensible, continuous descriptors - RACs

Based on autocorrelations

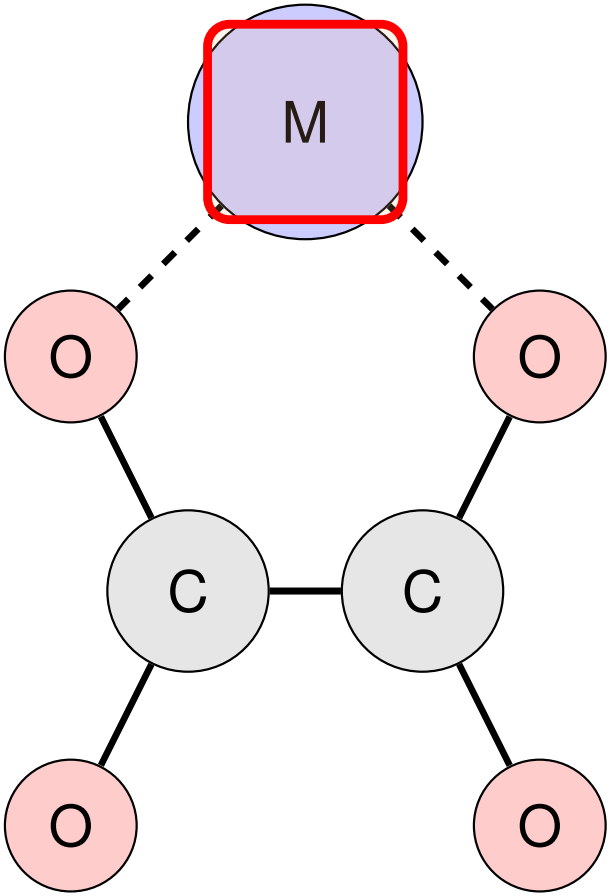


How to adapt to TM complexes?

restrict the scope to focus on *near-metal atoms*

Extensible, continuous descriptors - RACs

Based on autocorrelations

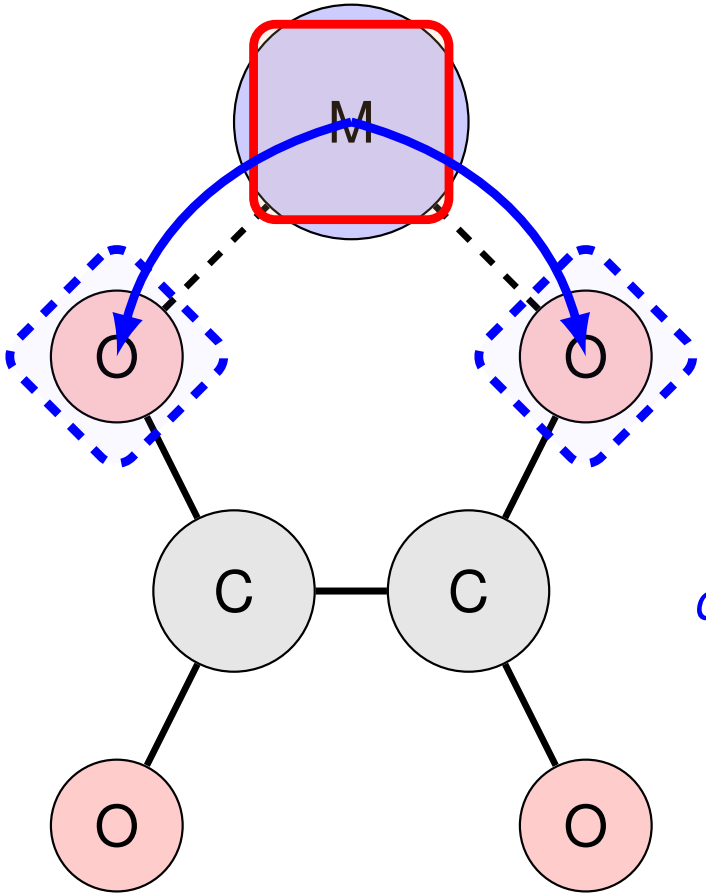


How to adapt to TM complexes?

restrict the scope to focus on *near-metal atoms*

Extensible, continuous descriptors - RACs

Based on autocorrelations



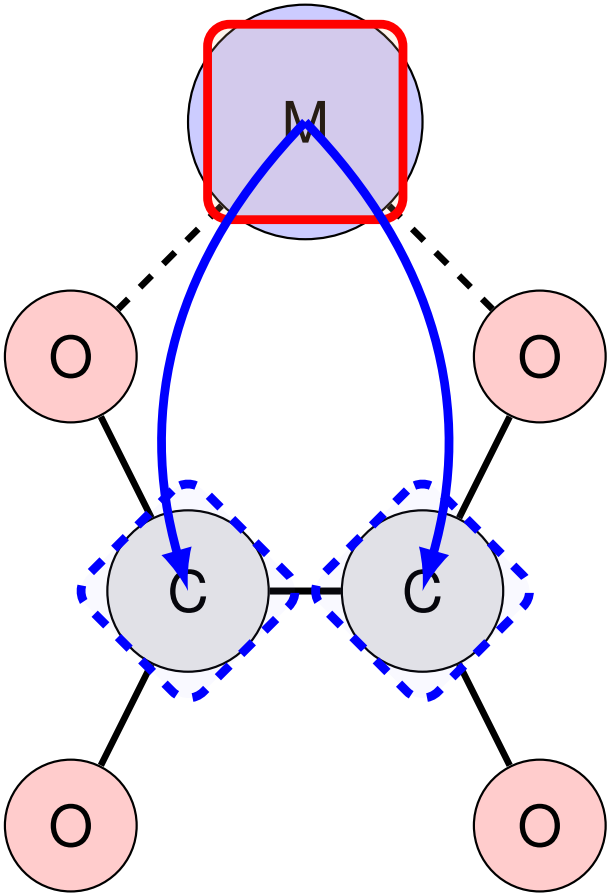
How to adapt to TM complexes?

restrict the scope to focus on *near-metal atoms*

$$d_1 : \sum_{M,O} Z_M Z_O$$

Extensible, continuous descriptors - RACs

Based on autocorrelations



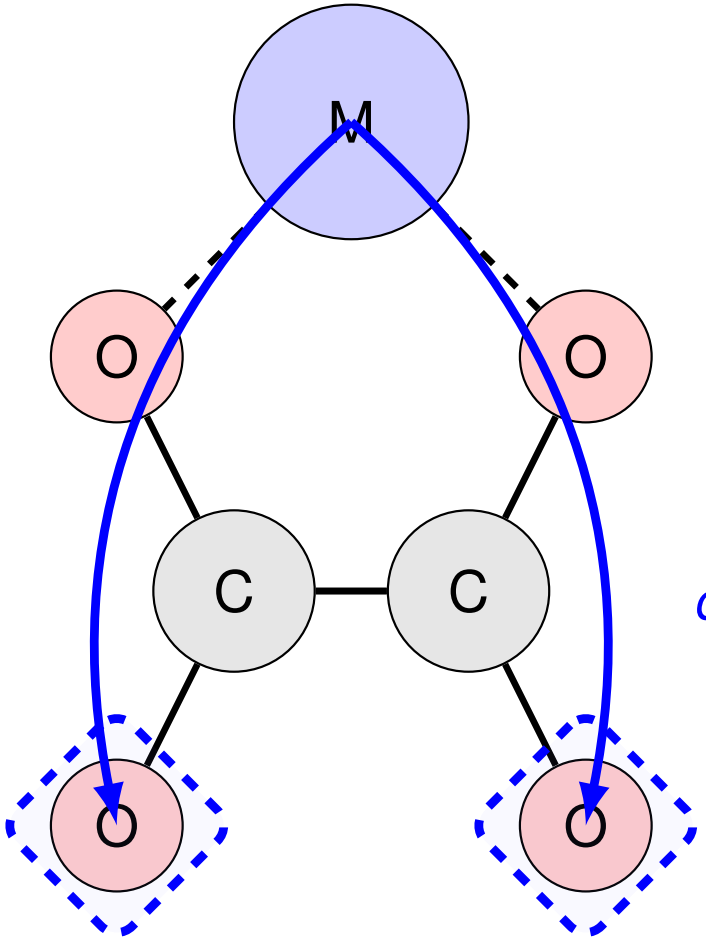
How to adapt to TM complexes?

restrict the scope to focus on *near-metal atoms*

$$d_2 : \sum_{M,C} Z_M Z_C$$

Extensible, continuous descriptors - RACs

Based on autocorrelations



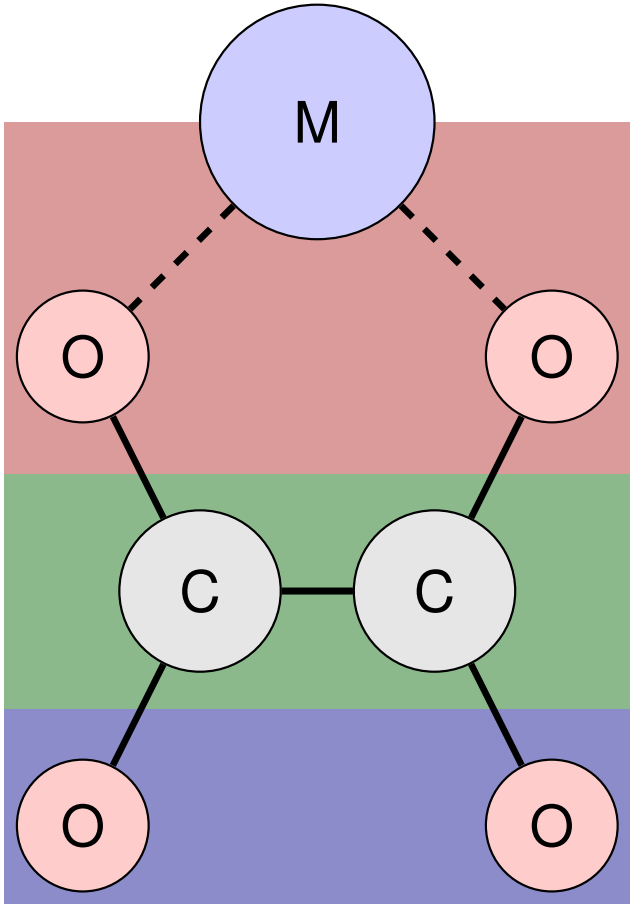
How to adapt to TM complexes?

restrict the scope to focus on *near-metal atoms*

$$d_3 : \sum_{M,O} Z_M Z_O$$

Extensible, continuous descriptors - RACs

Based on autocorrelations



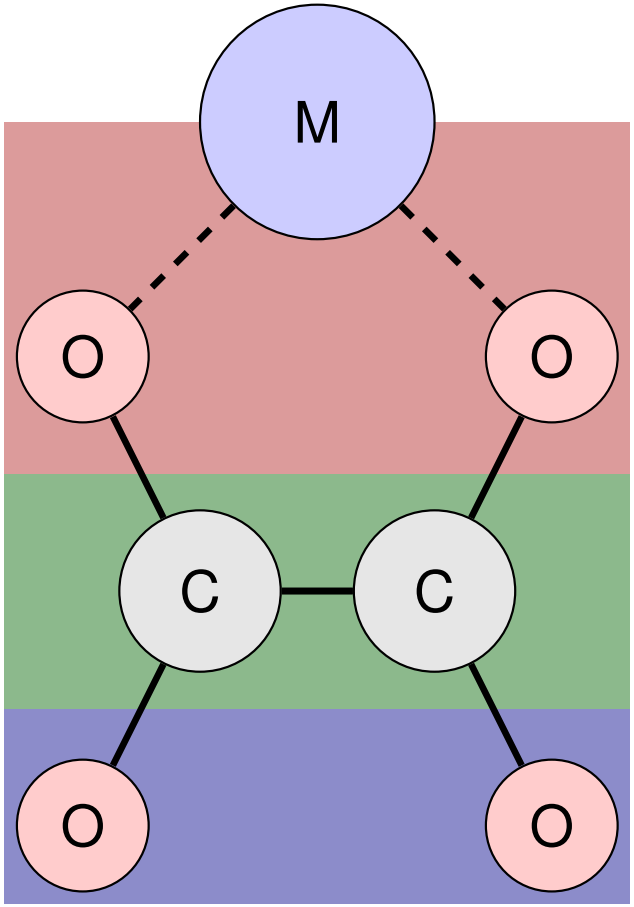
How to adapt to TM complexes?

restrict the scope to focus on *near-metal atoms*

$$d_3 : \sum_{M,O} Z_M Z_O$$

Extensible, continuous descriptors - RACs

Based on autocorrelations



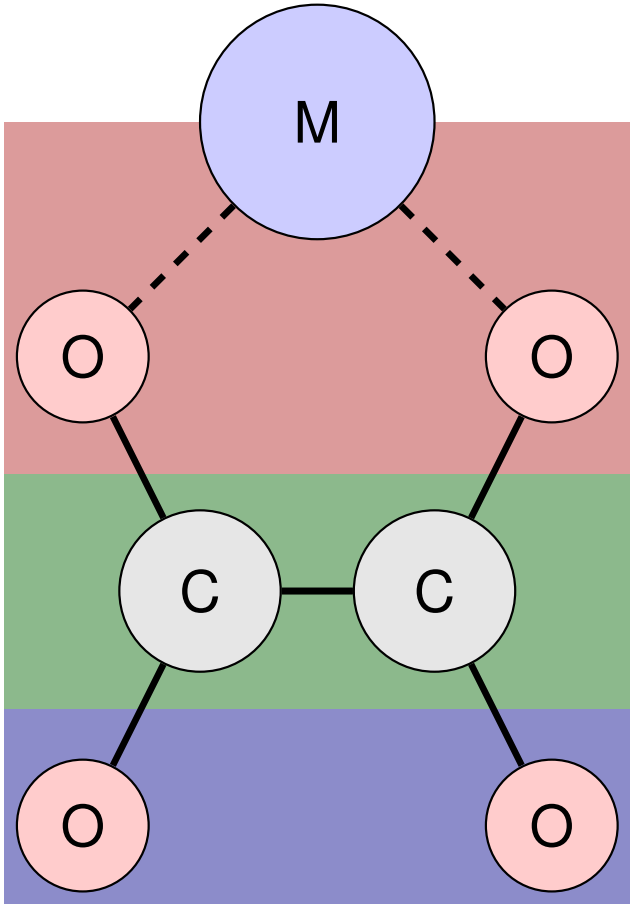
How to adapt to TM complexes?

restrict the scope to focus on *near-metal atoms*

$$d_3 : \sum_{M,O} Z_M Z_O \left(Z_i - Z_j\right)$$

Extensible, continuous descriptors - RACs

Based on autocorrelations



How to adapt to TM complexes?

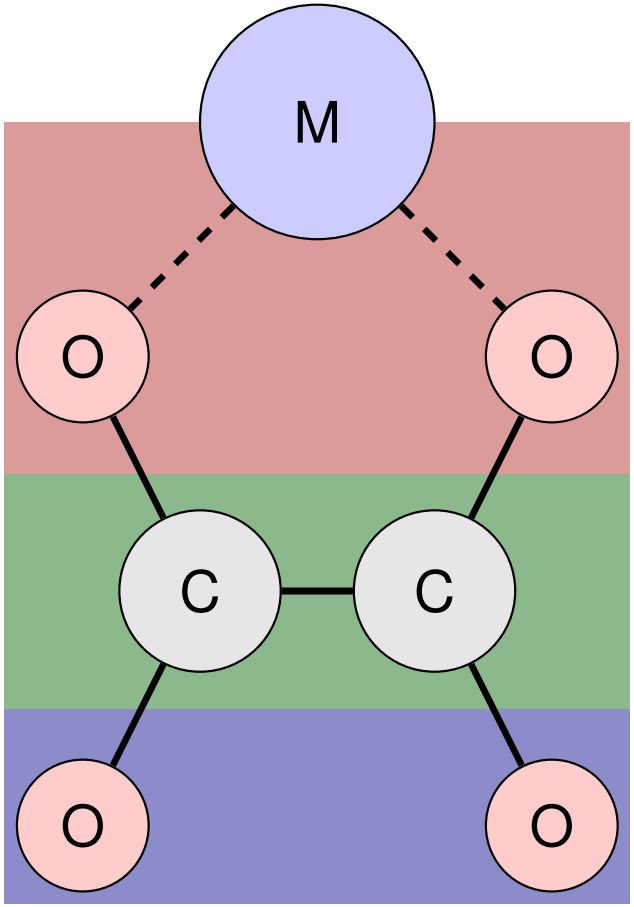
restrict the scope to focus on *near-metal atoms*

$$d_3 : \sum_{M,O} Z_M Z_O \left(Z_i - Z_j\right)$$

properties: T, χ, Z, I, S

Extensible, continuous descriptors - RACs

Based on autocorrelations



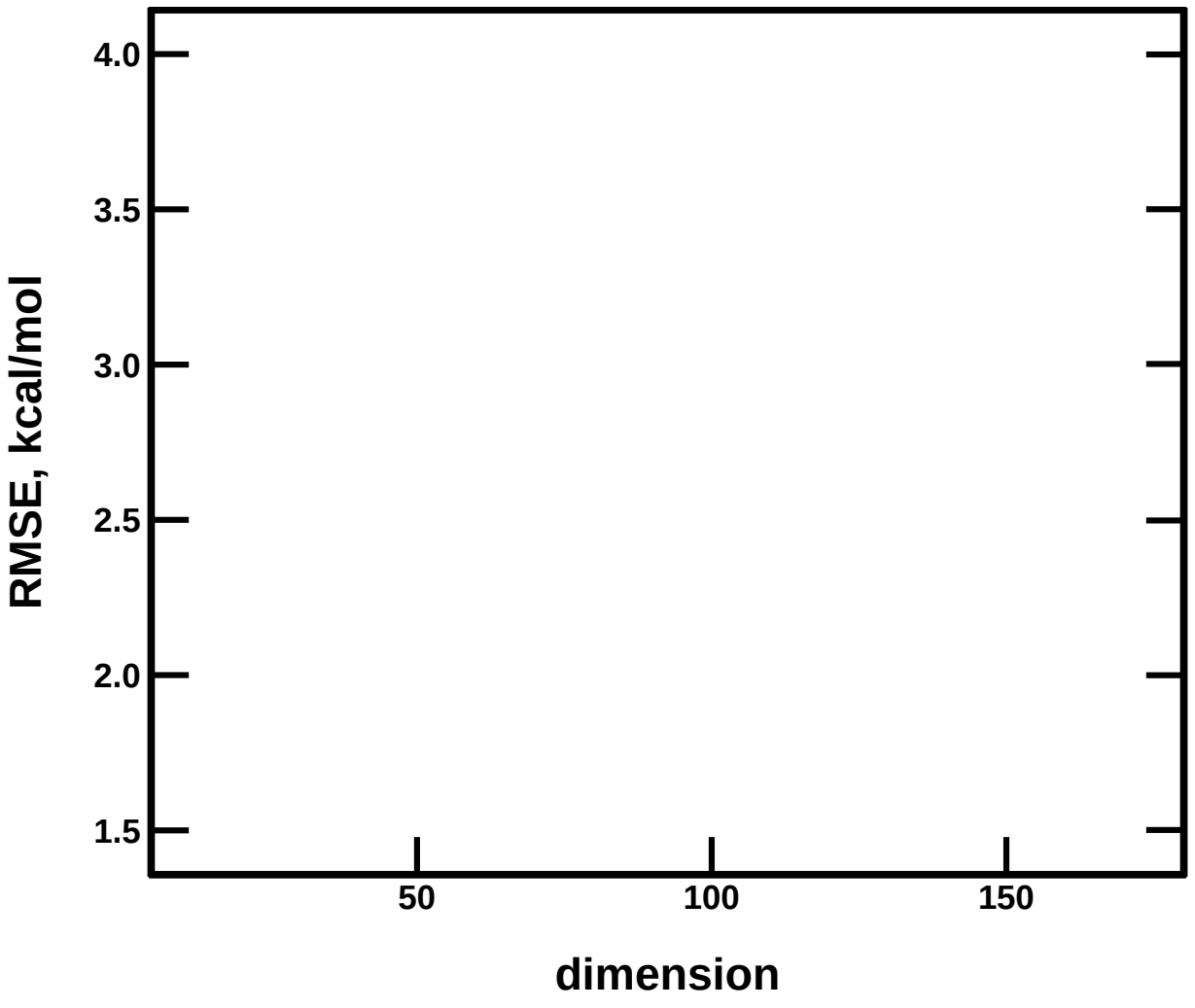
How to adapt to TM complexes?

restrict the scope to focus on *near-metal atoms*

$$d_3 : \sum_{M,O} Z_M Z_O \left(Z_i - Z_j\right)$$

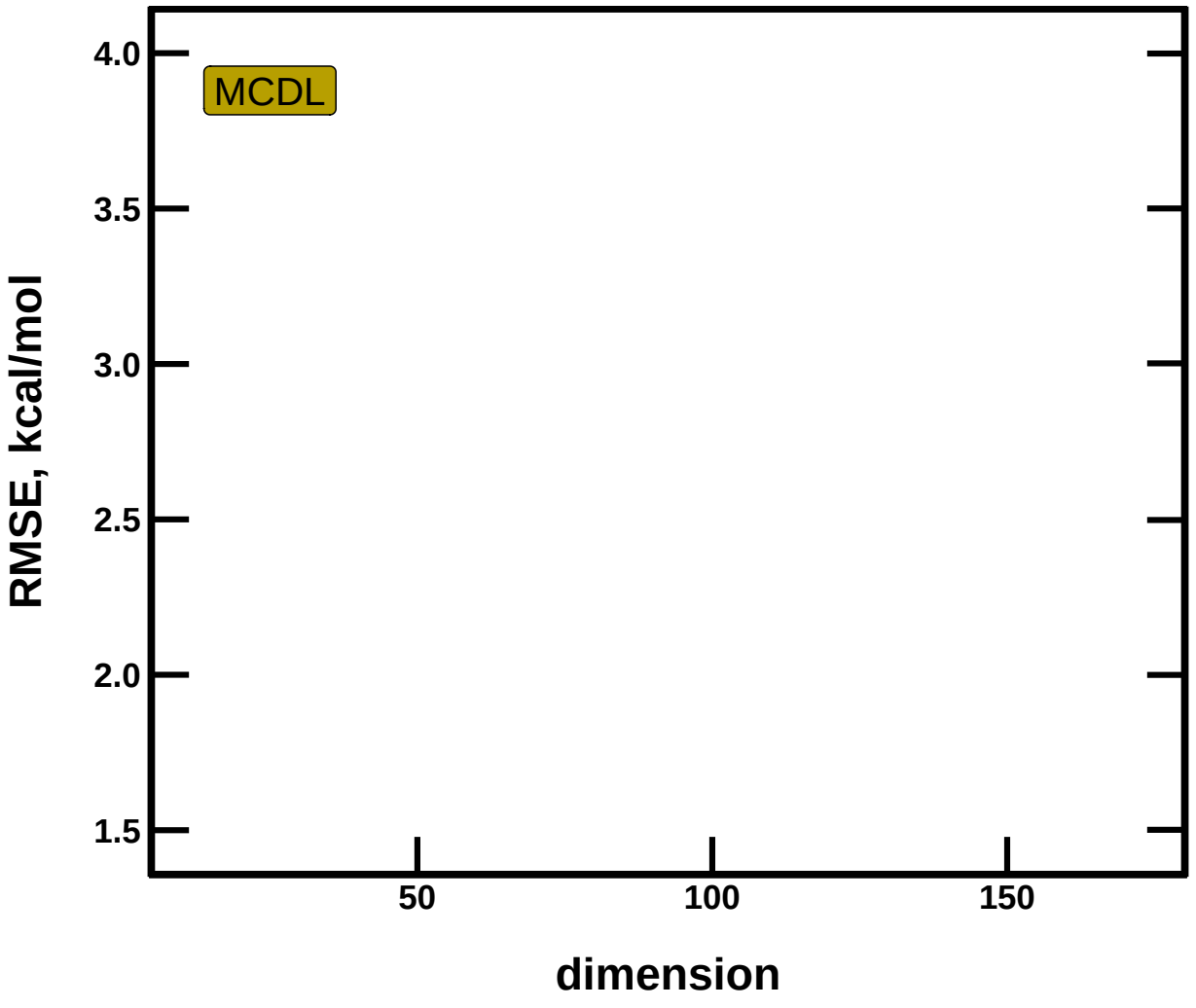
$\sim$ 160 features in total

Feature selection



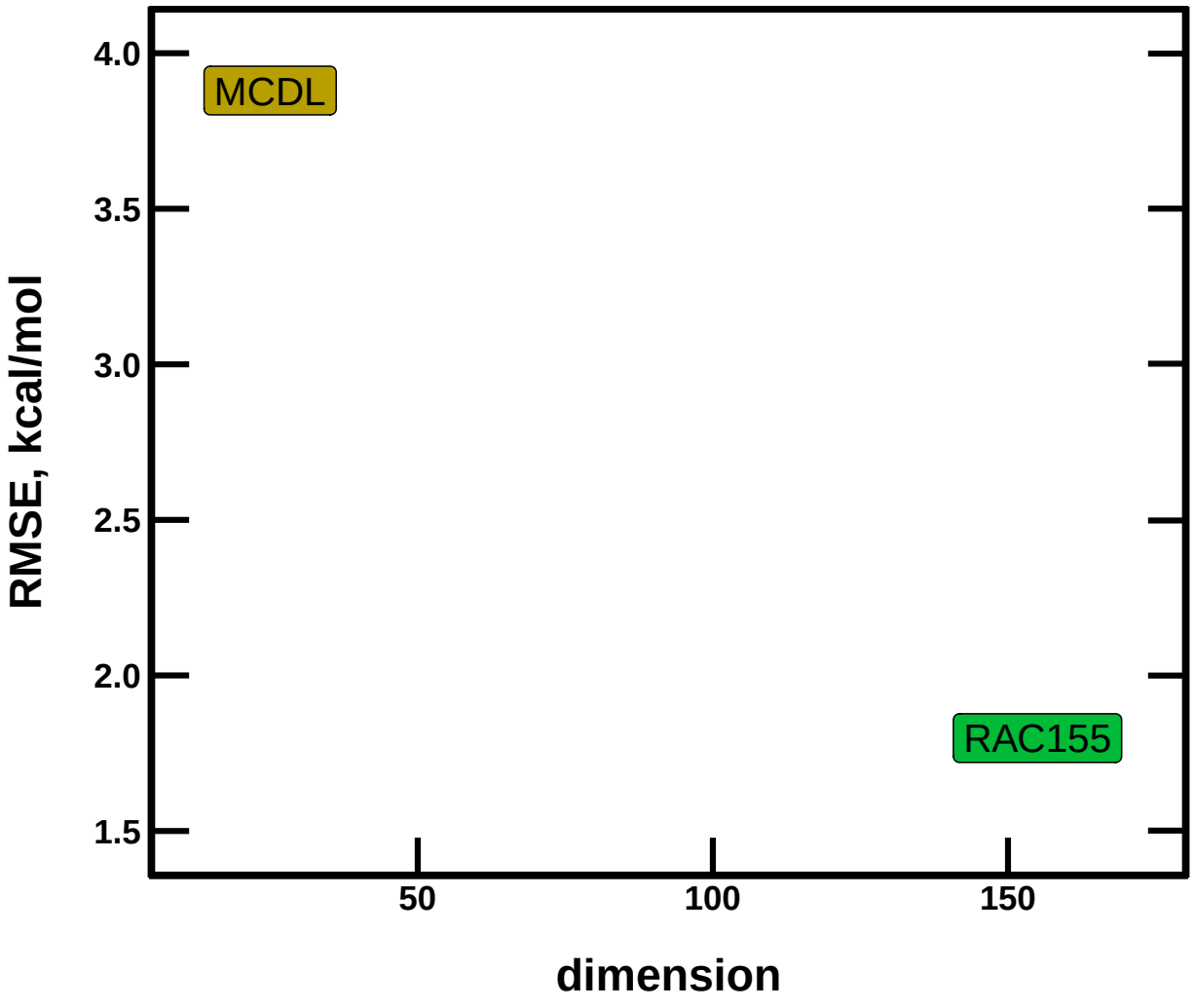
Janet, J.P., and Kulik, H.J. *J. Phys. Chem. A*, 2017,121, 46, 8939-8954.

Feature selection



Janet, J.P., and Kulik, H.J. *J. Phys. Chem. A*, 2017,121, 46, 8939-8954.

Feature selection



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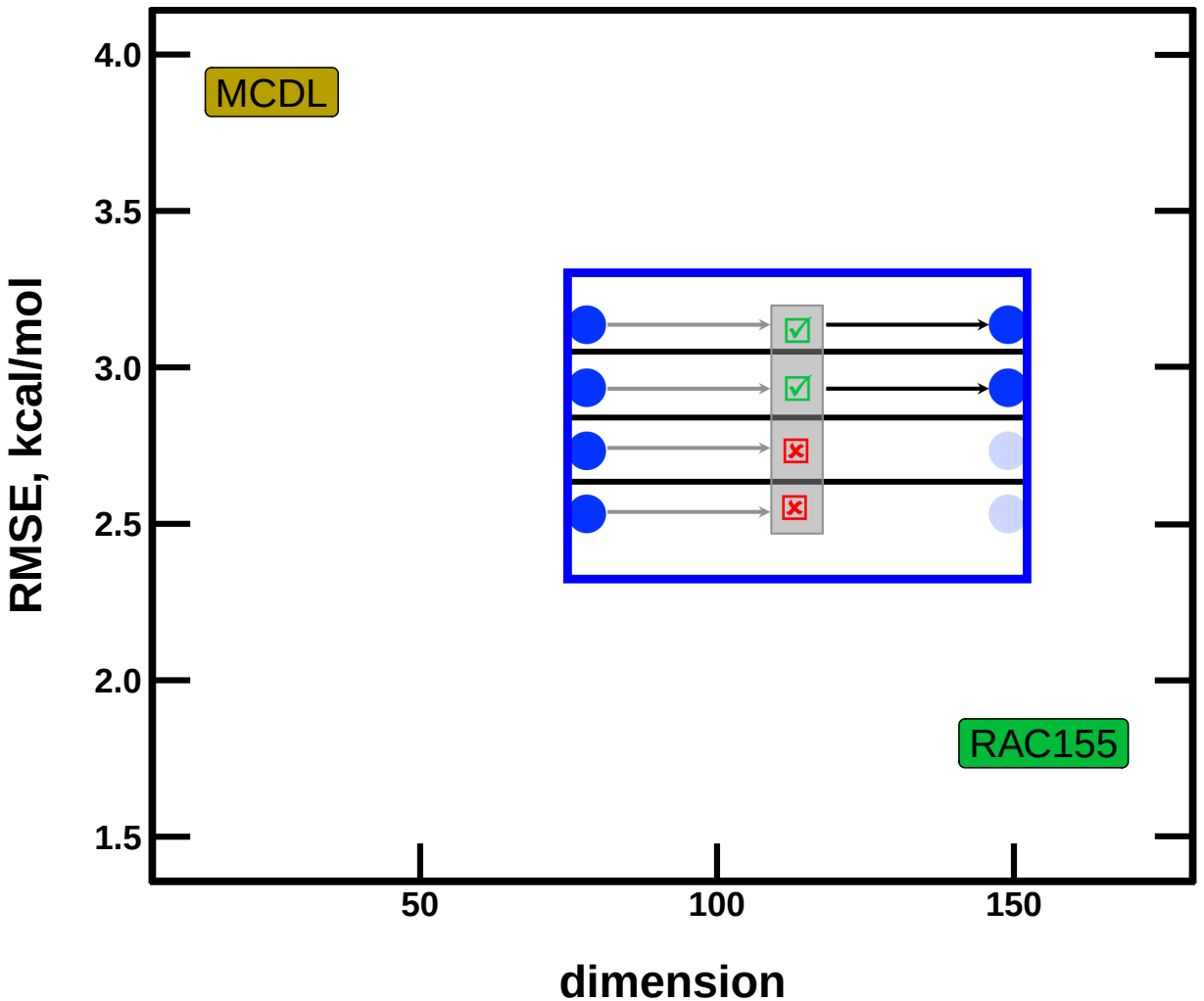

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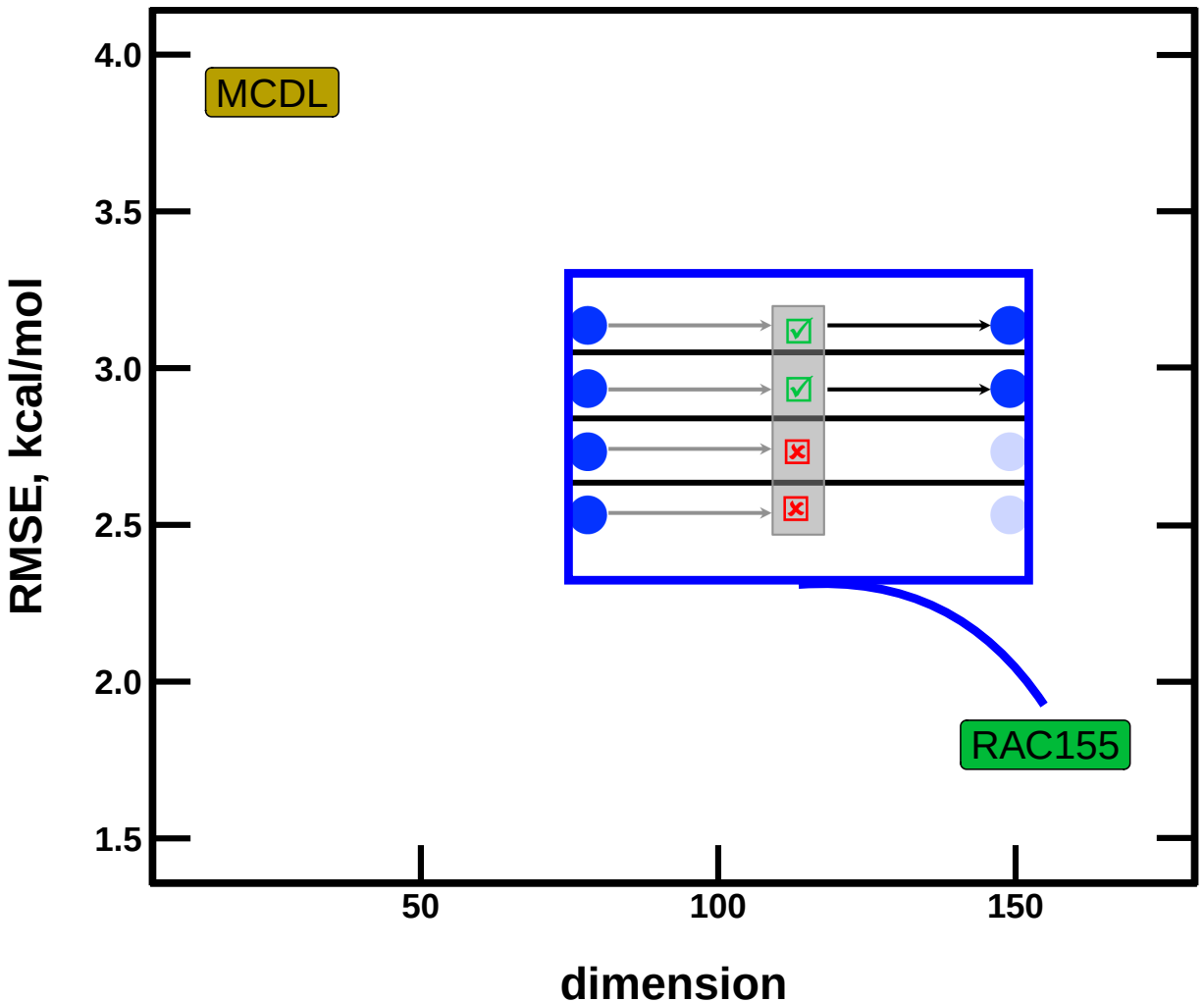

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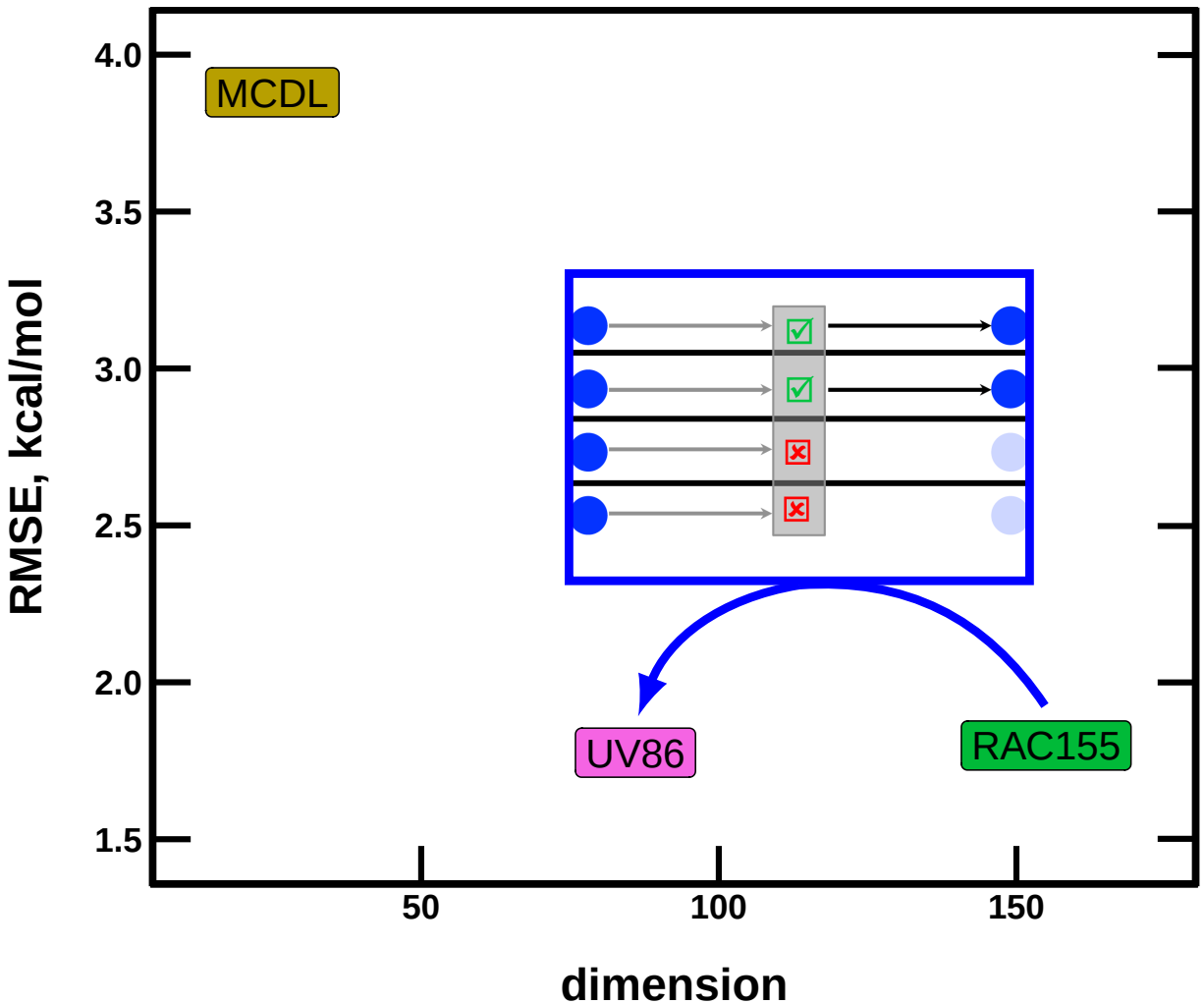

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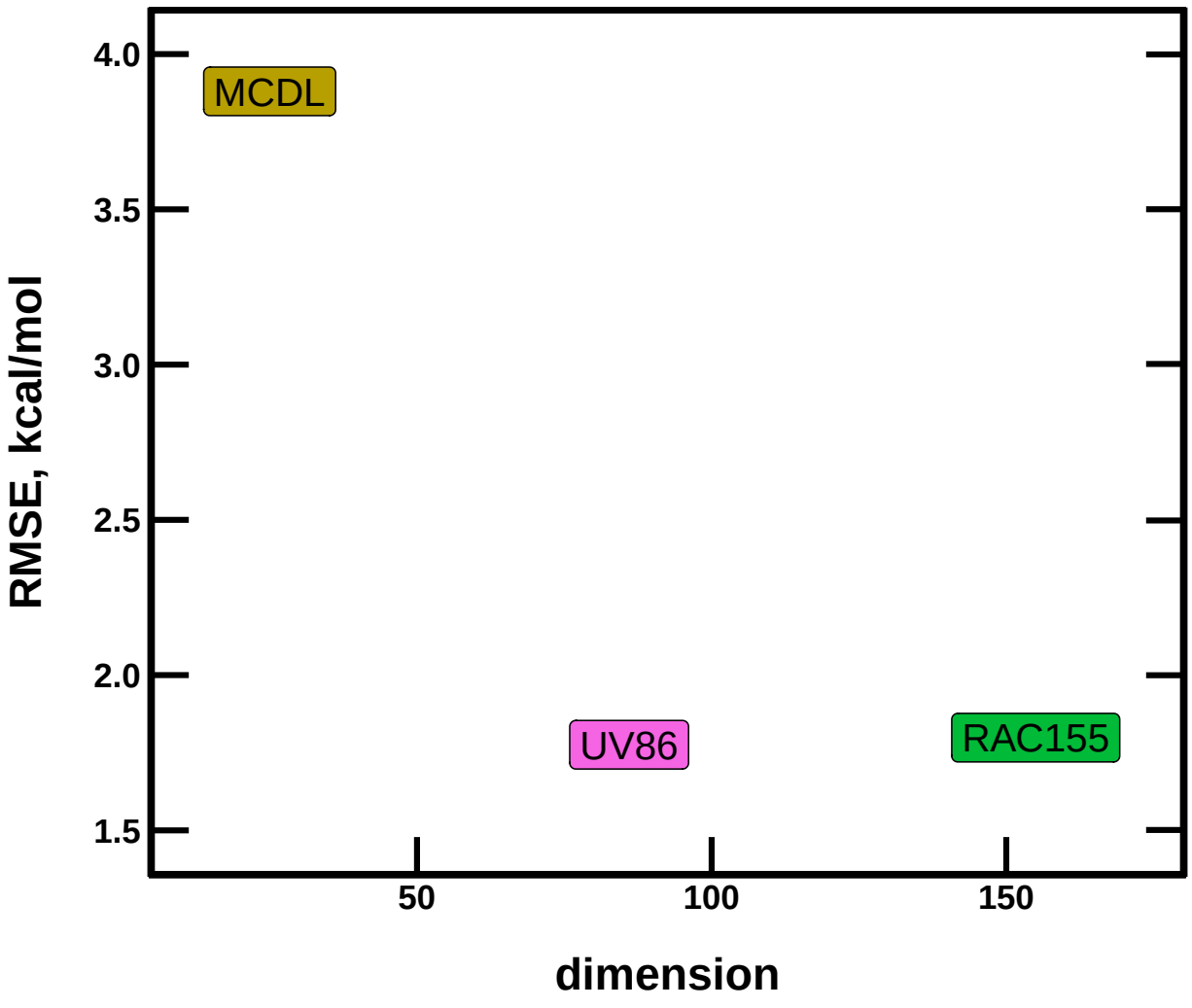

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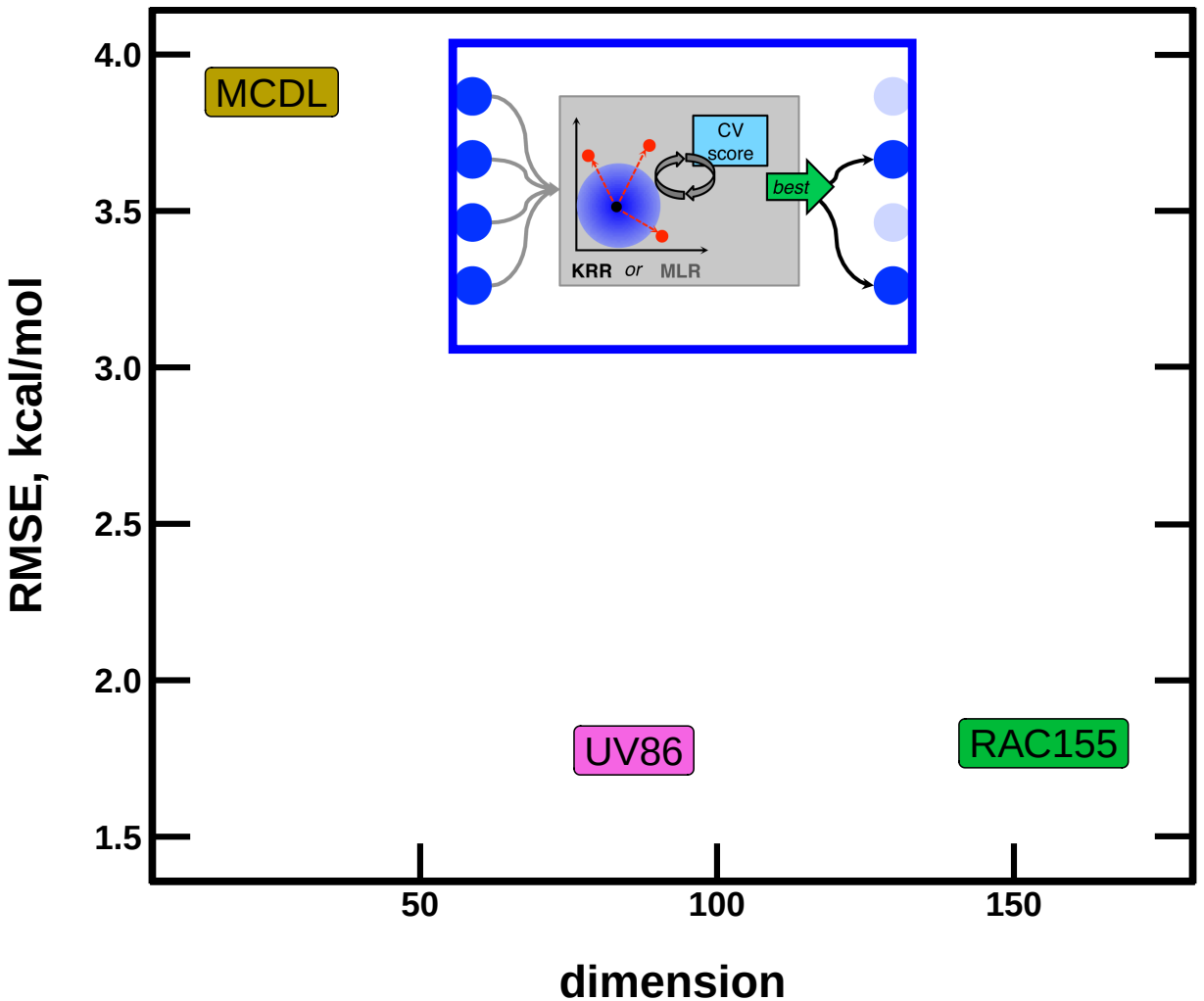
Feature selection



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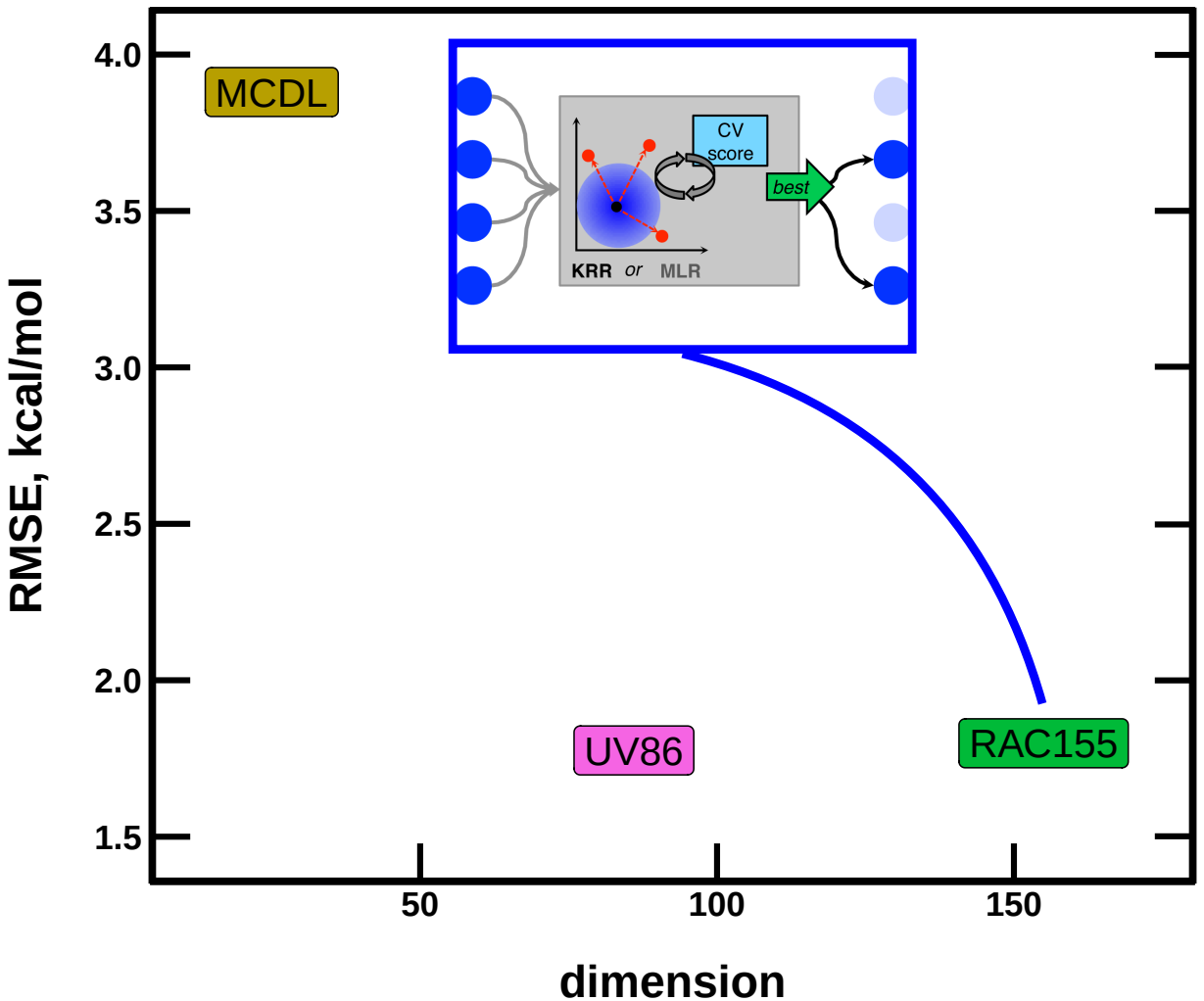

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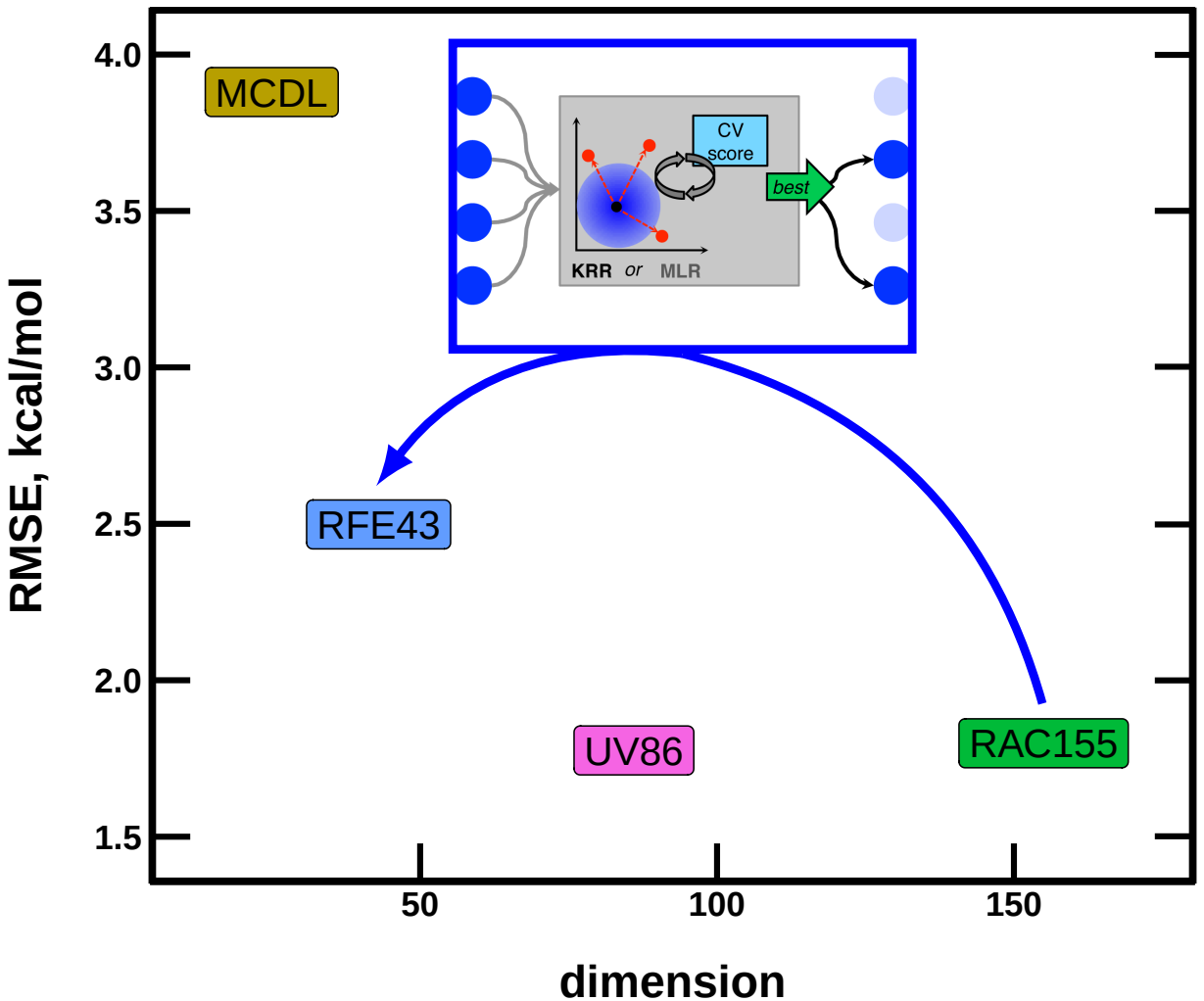

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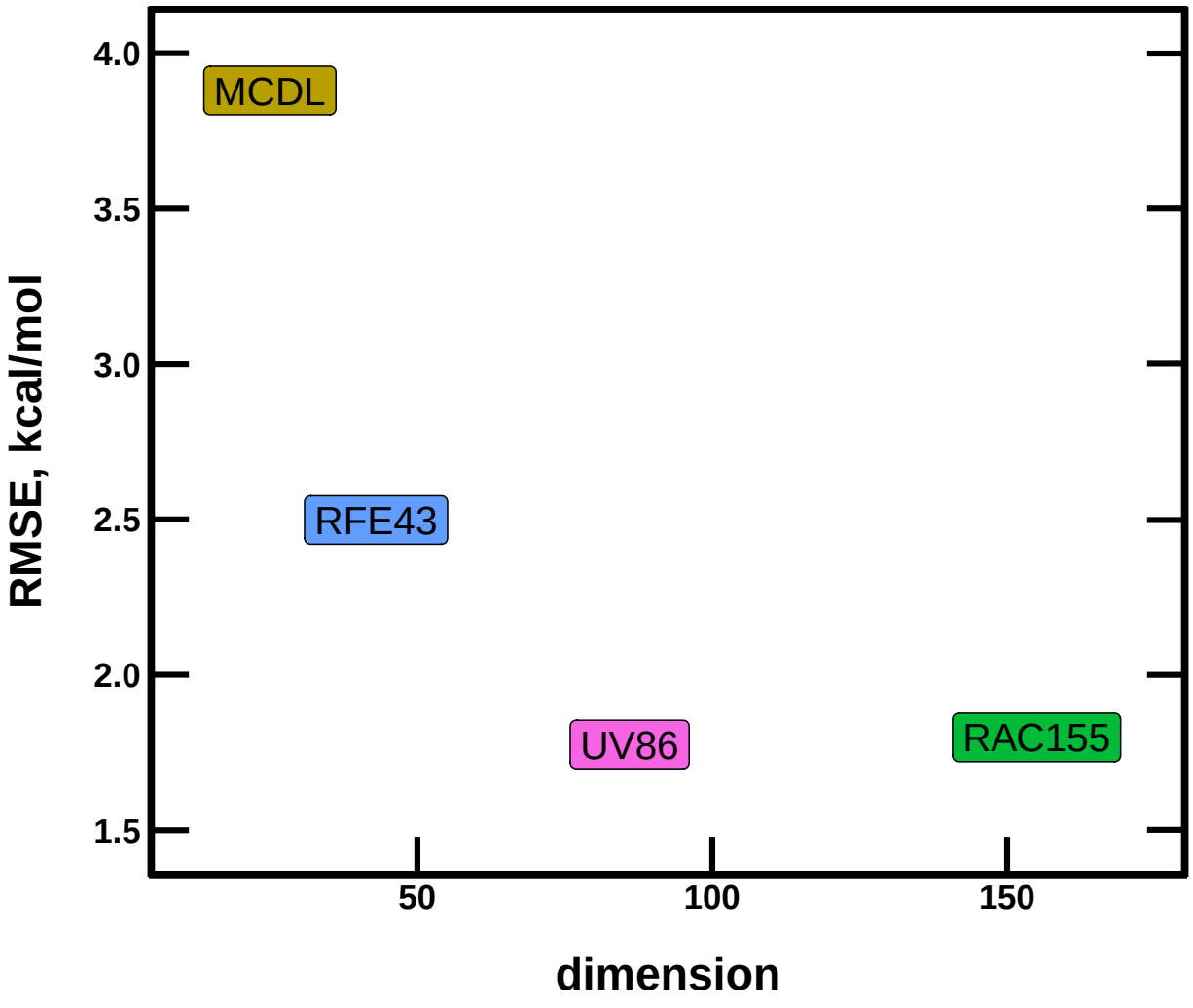

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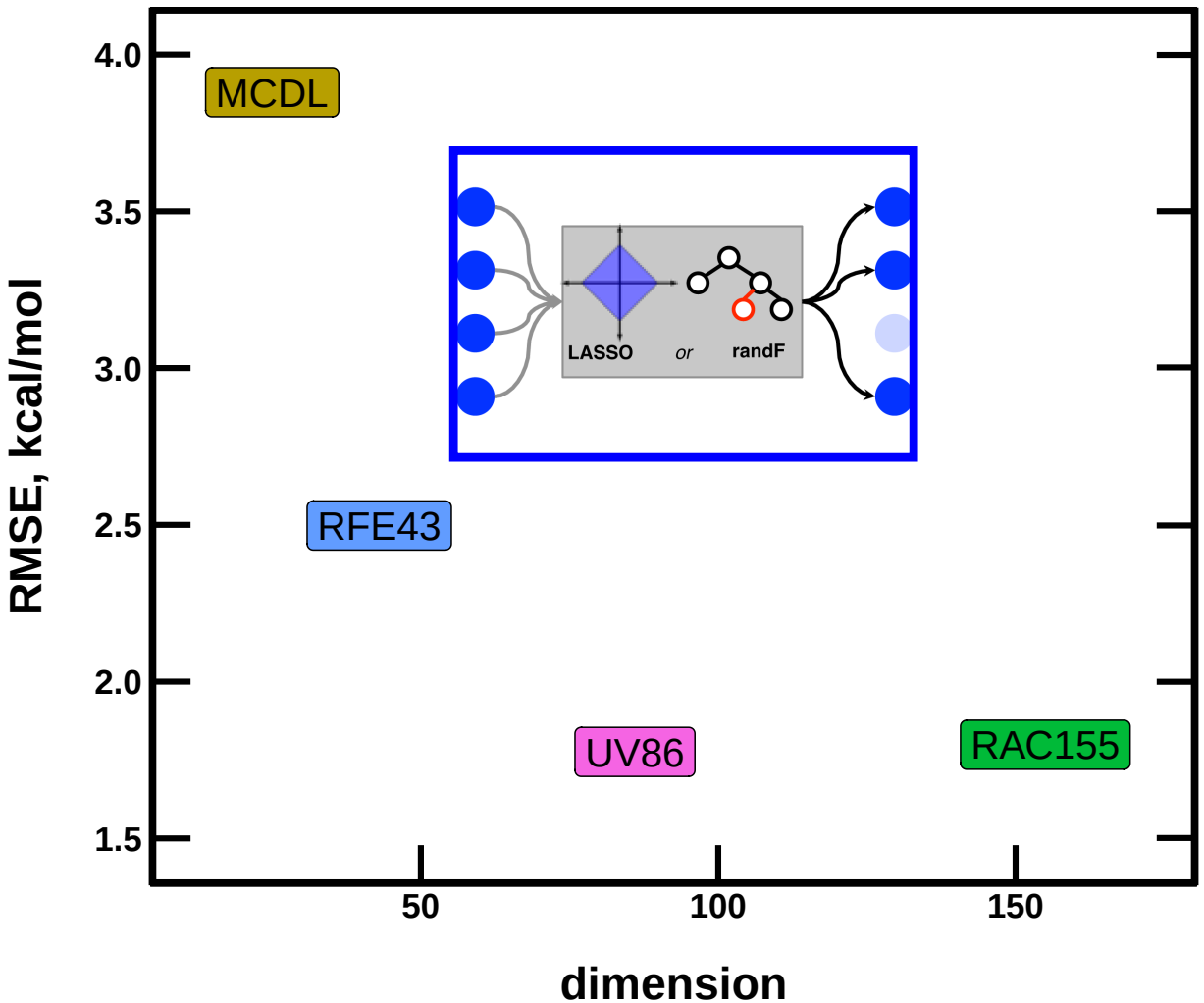

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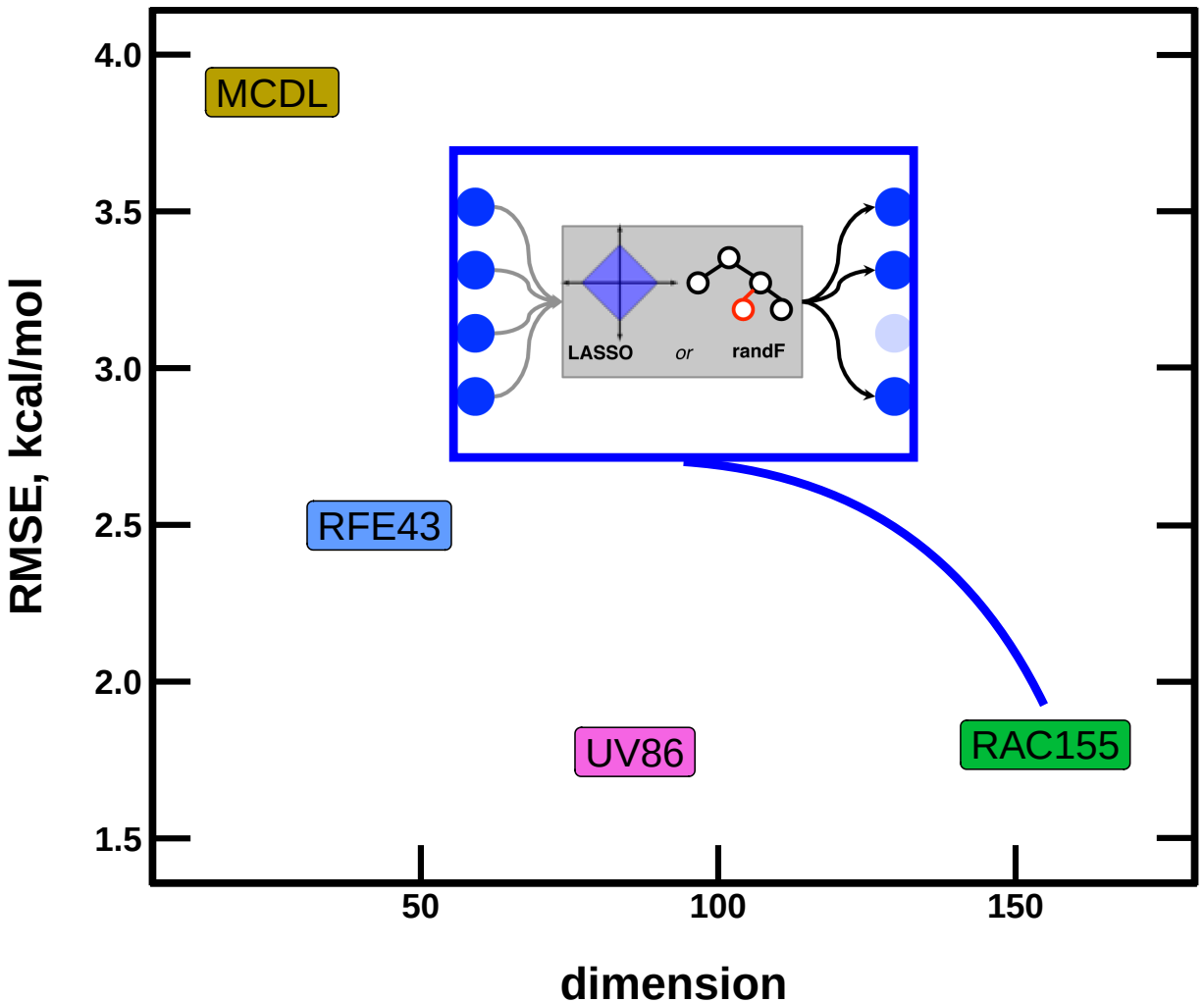

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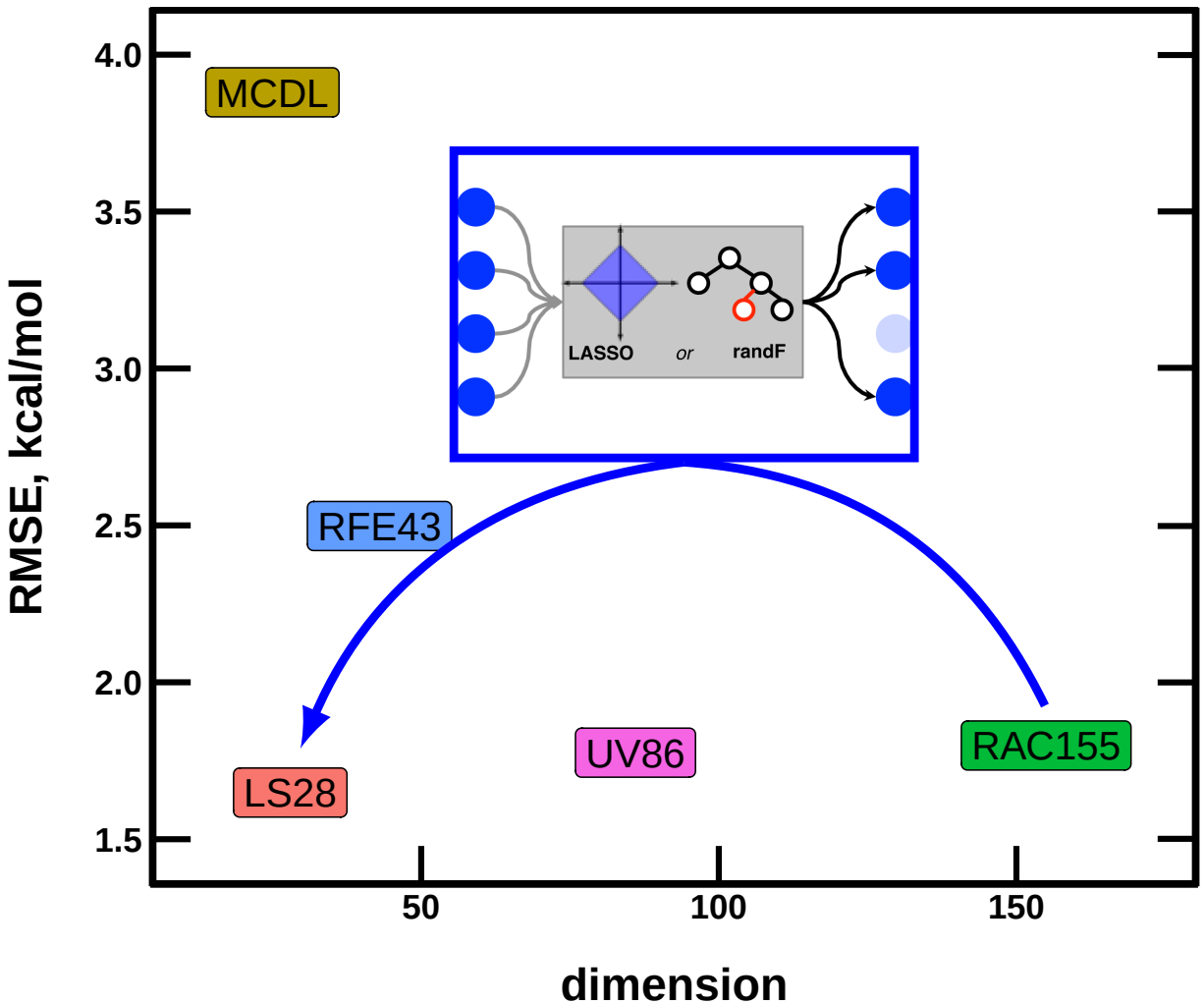
Feature selection



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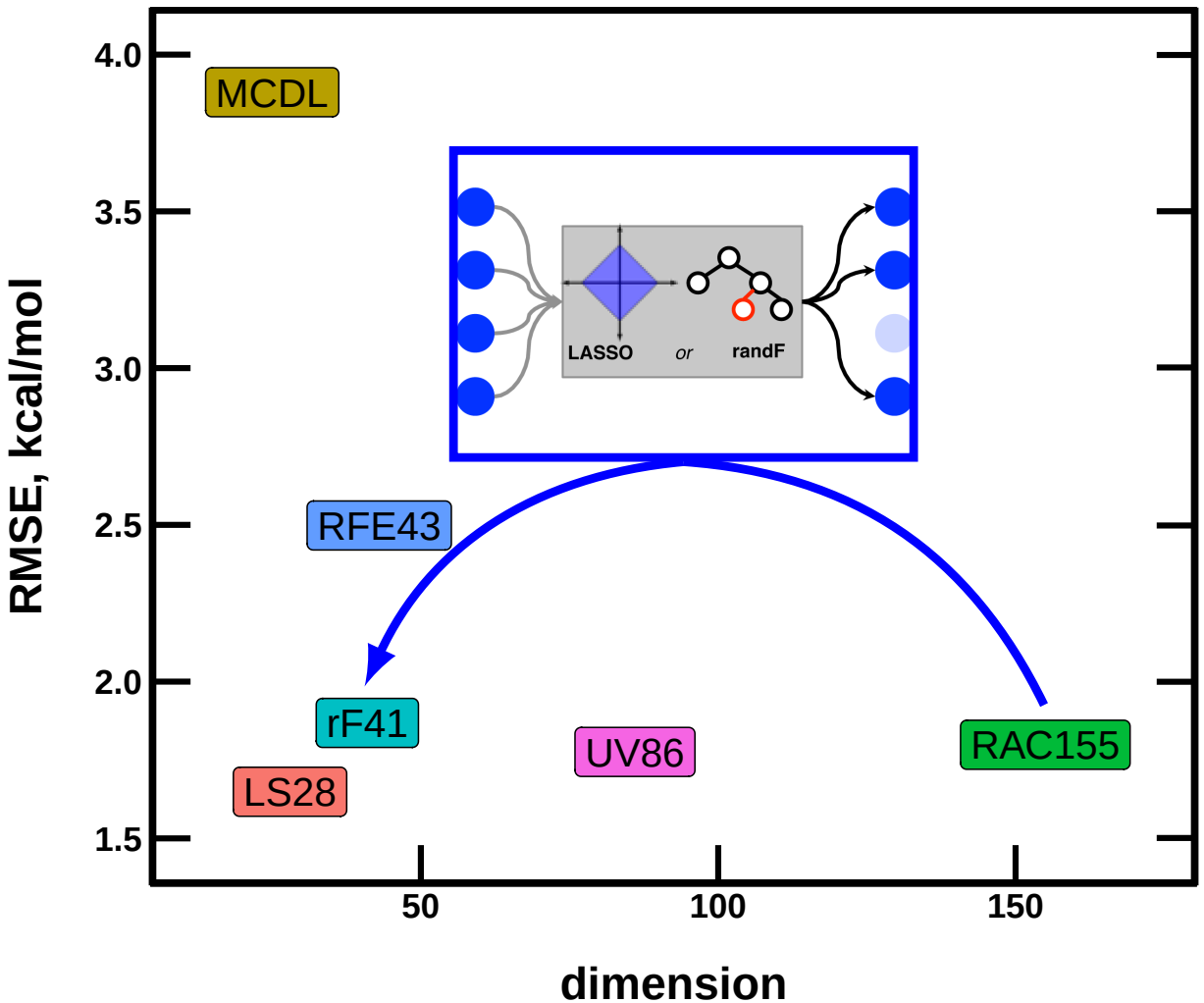
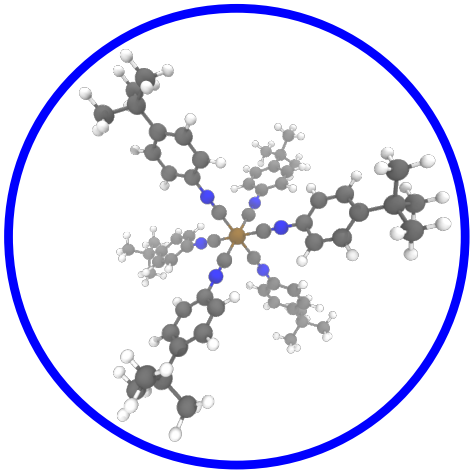
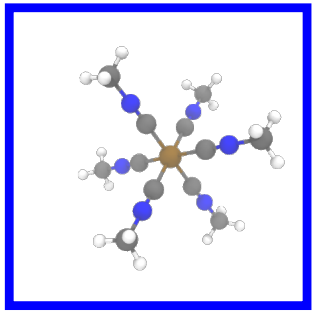
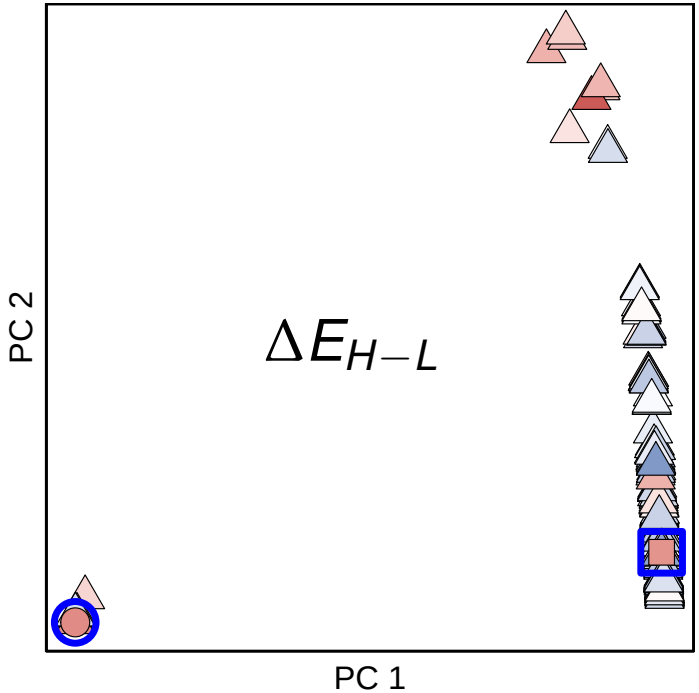


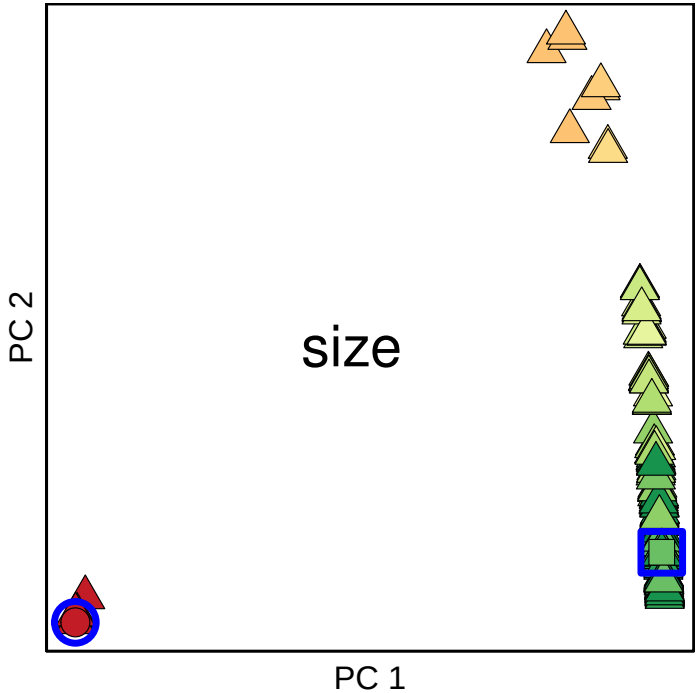
Janet, J.P., and Kulik, H.J. *J. Phys. Chem. A*, 2017,121, 46, 8939-8954.

A tale of two complexes, II

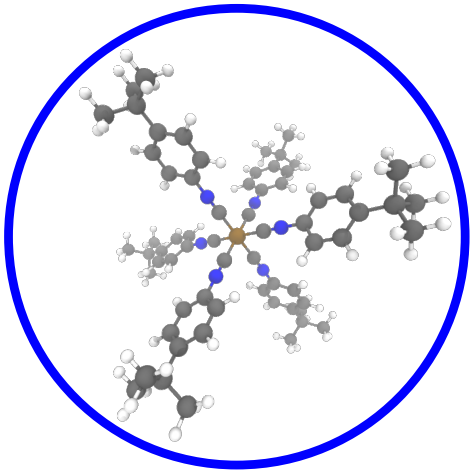


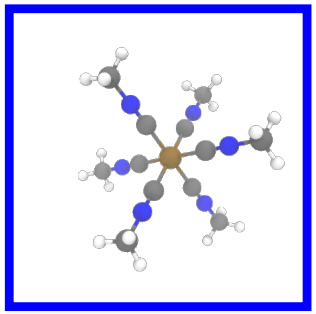


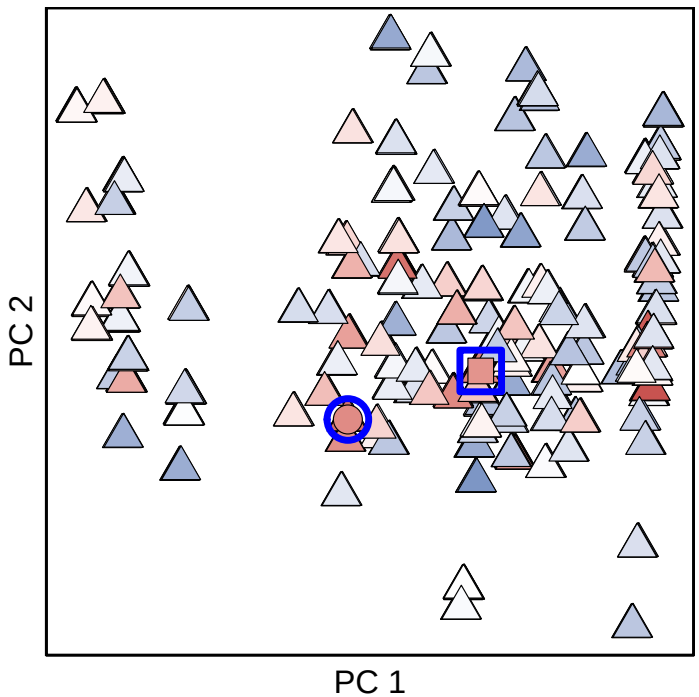


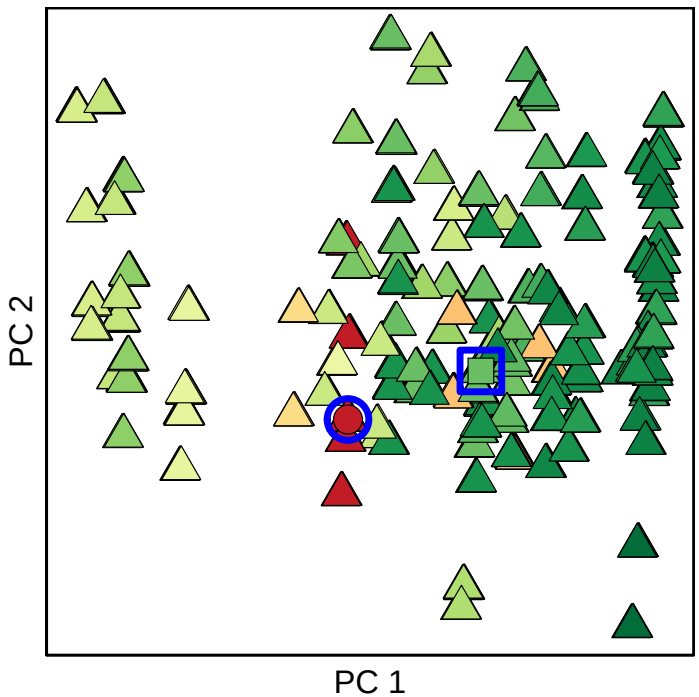


A tale of two complexes, II

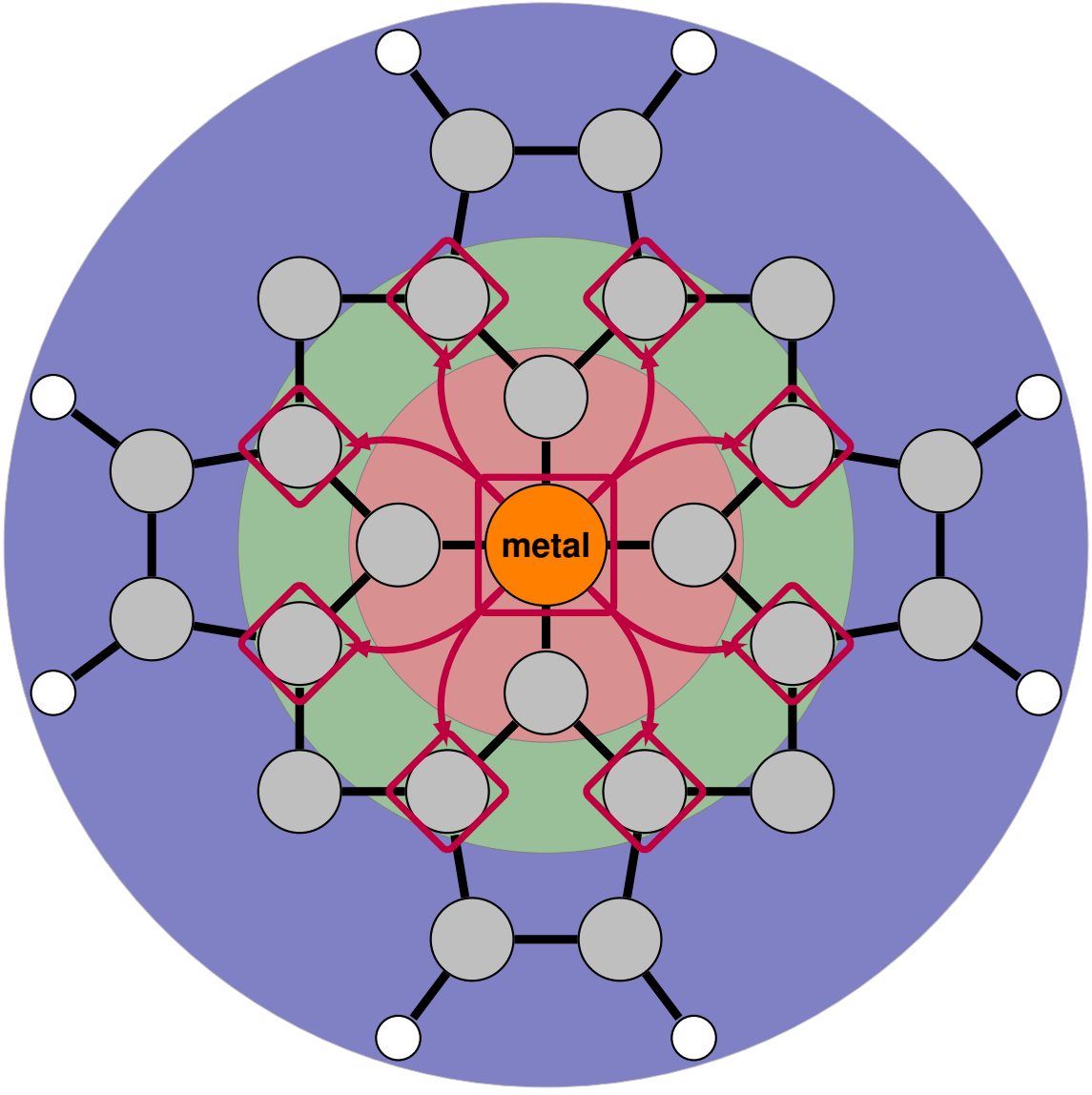




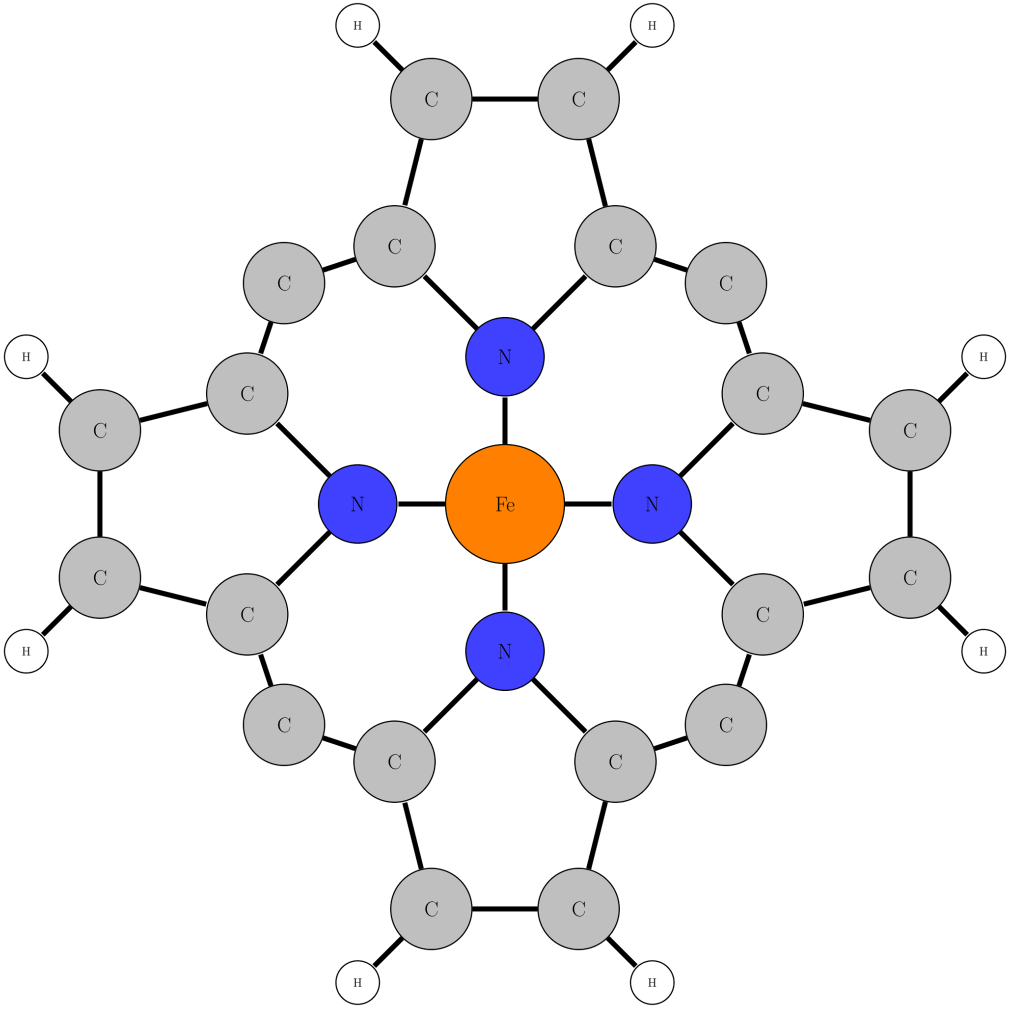




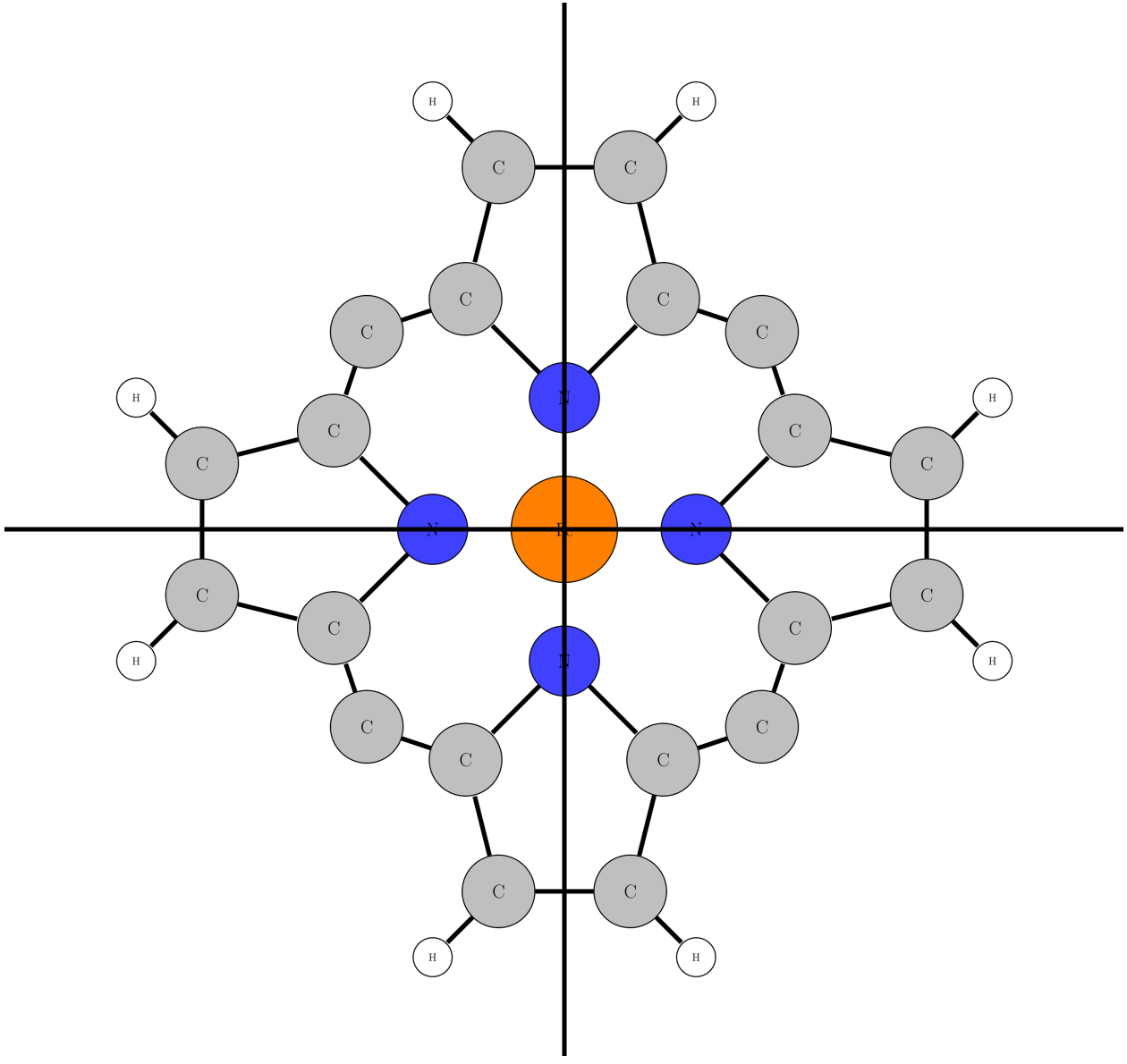
Do features depend on properties?



Do features depend on properties?

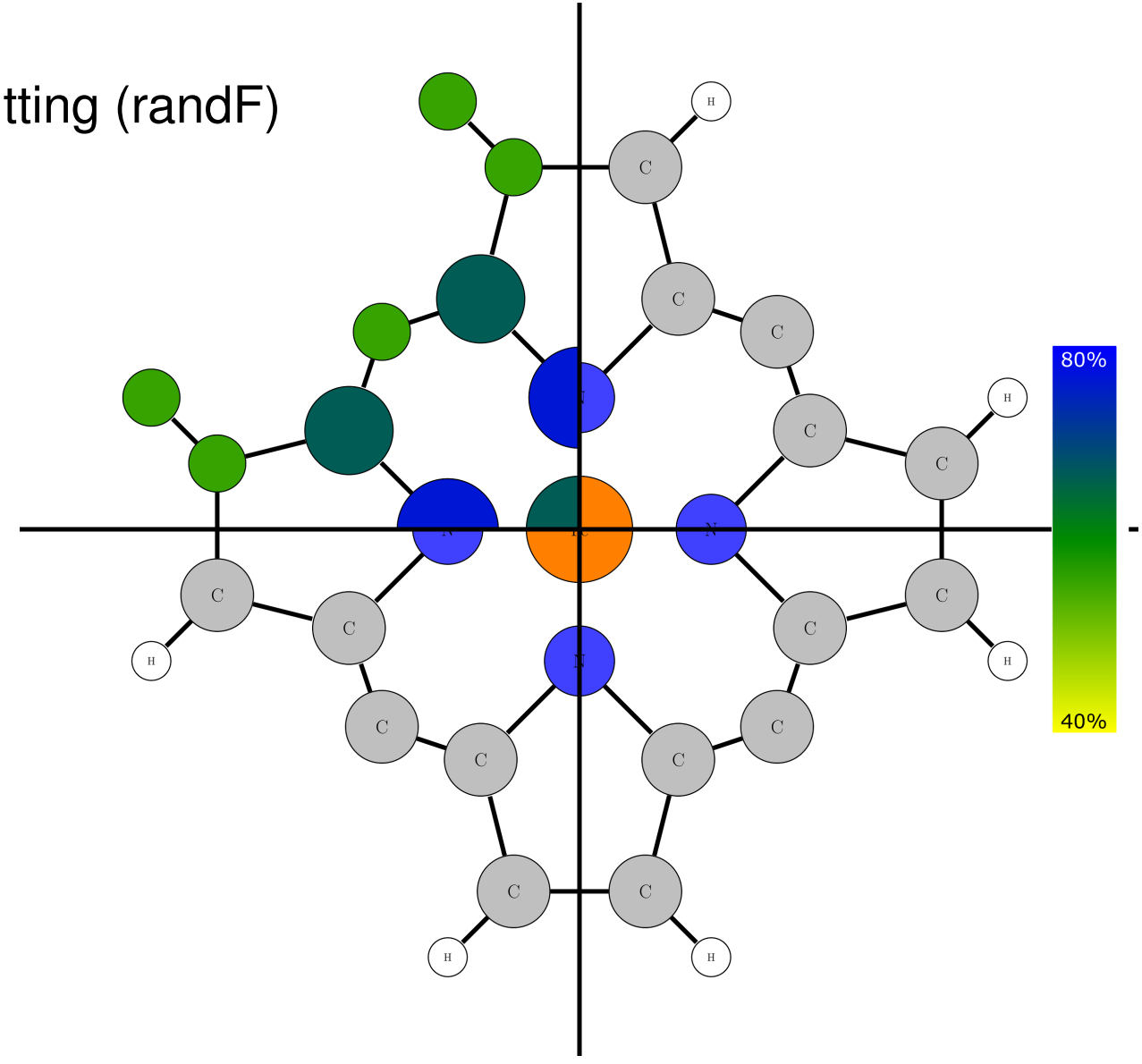


Do features depend on properties?

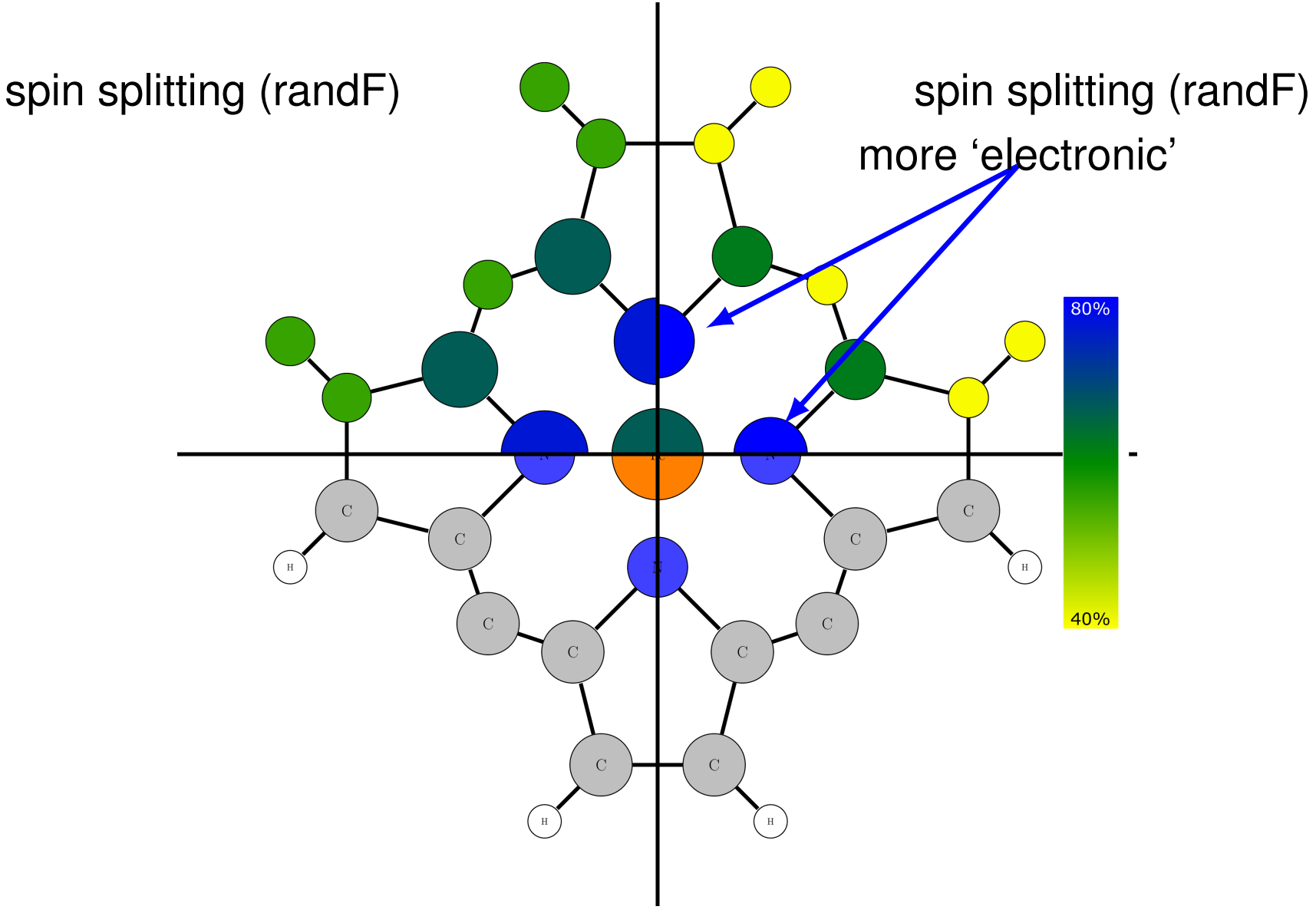


Do features depend on properties?

spin splitting (randF)



Do features depend on properties?



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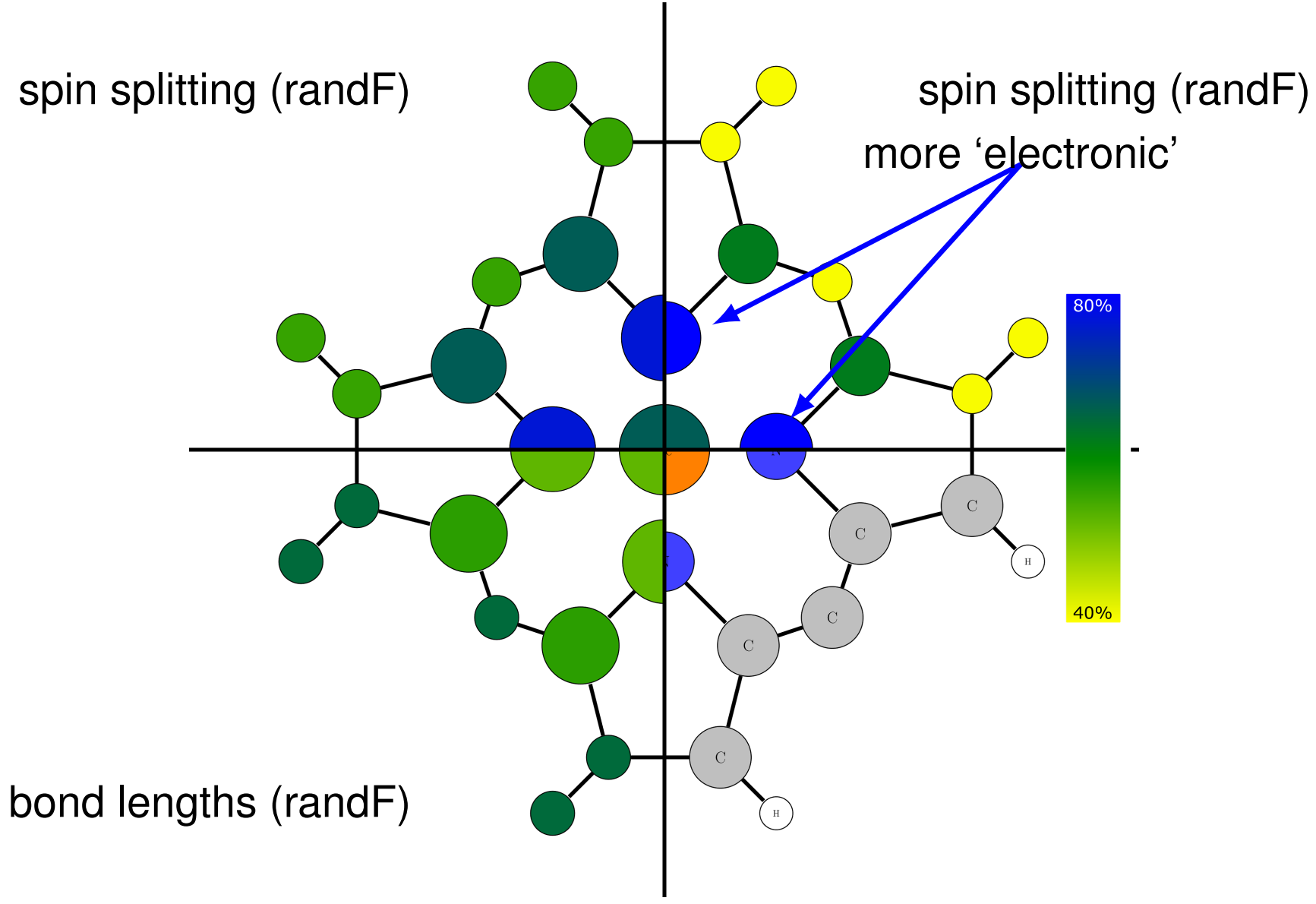

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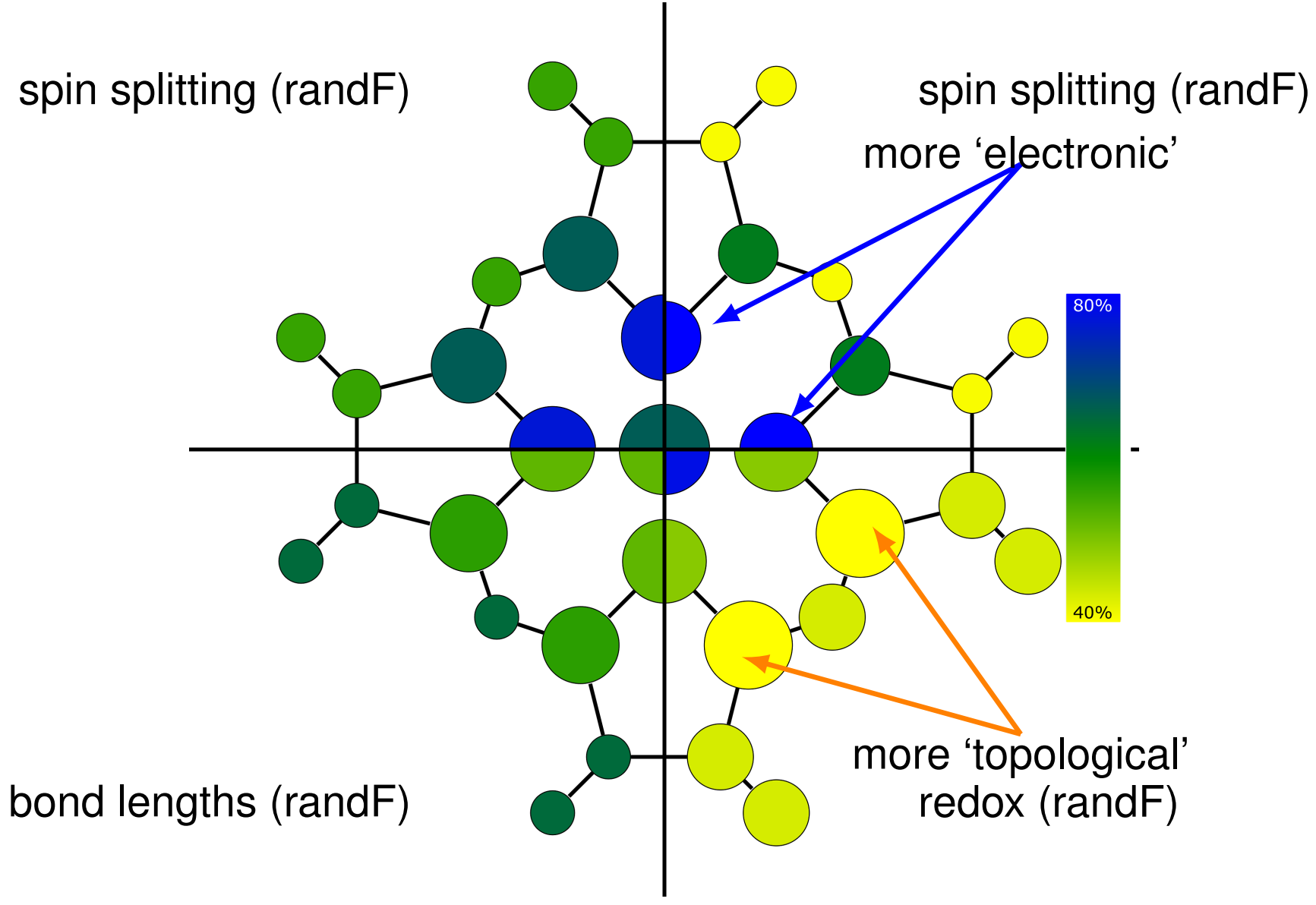
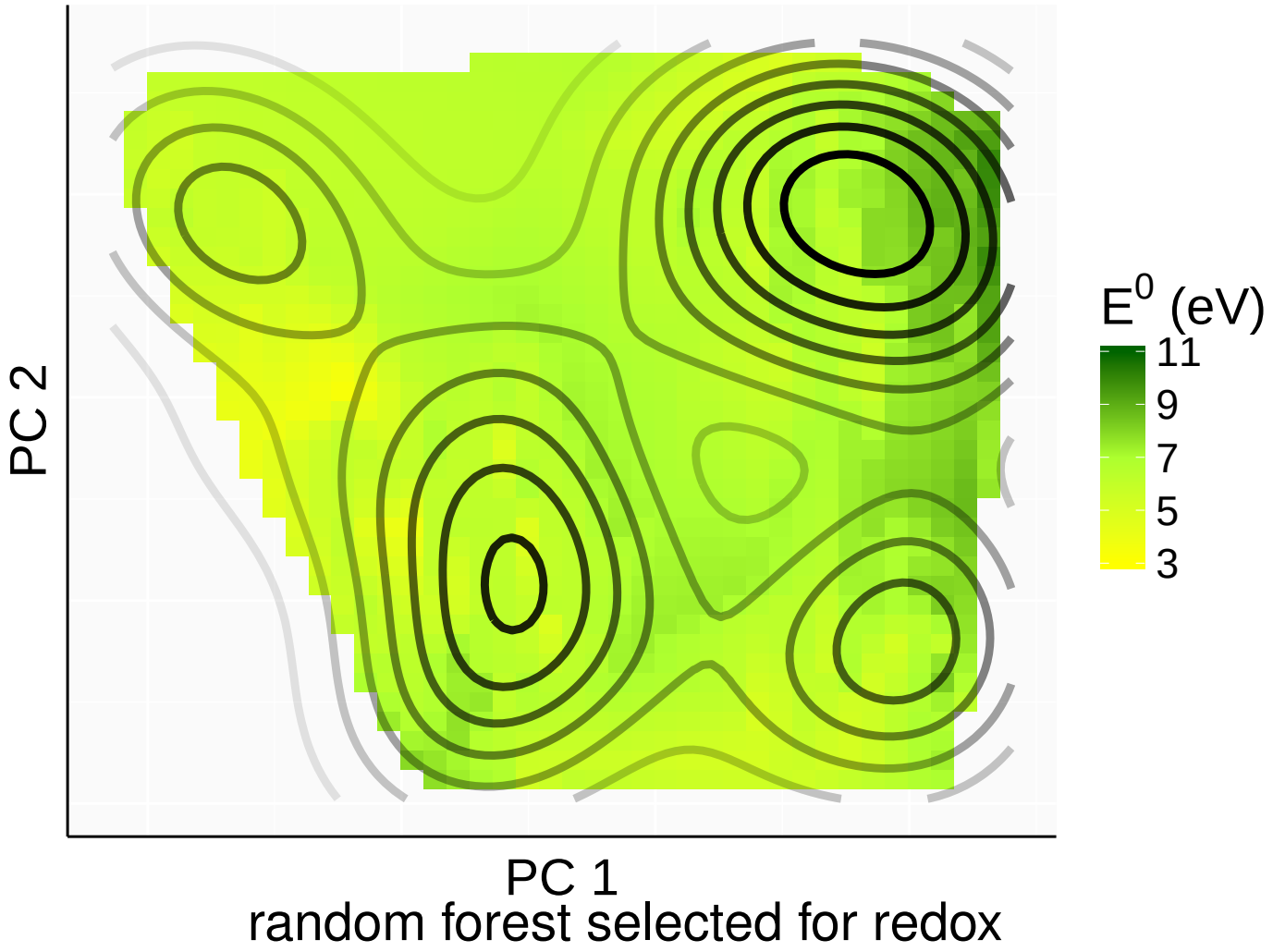


Mapping TM complex space



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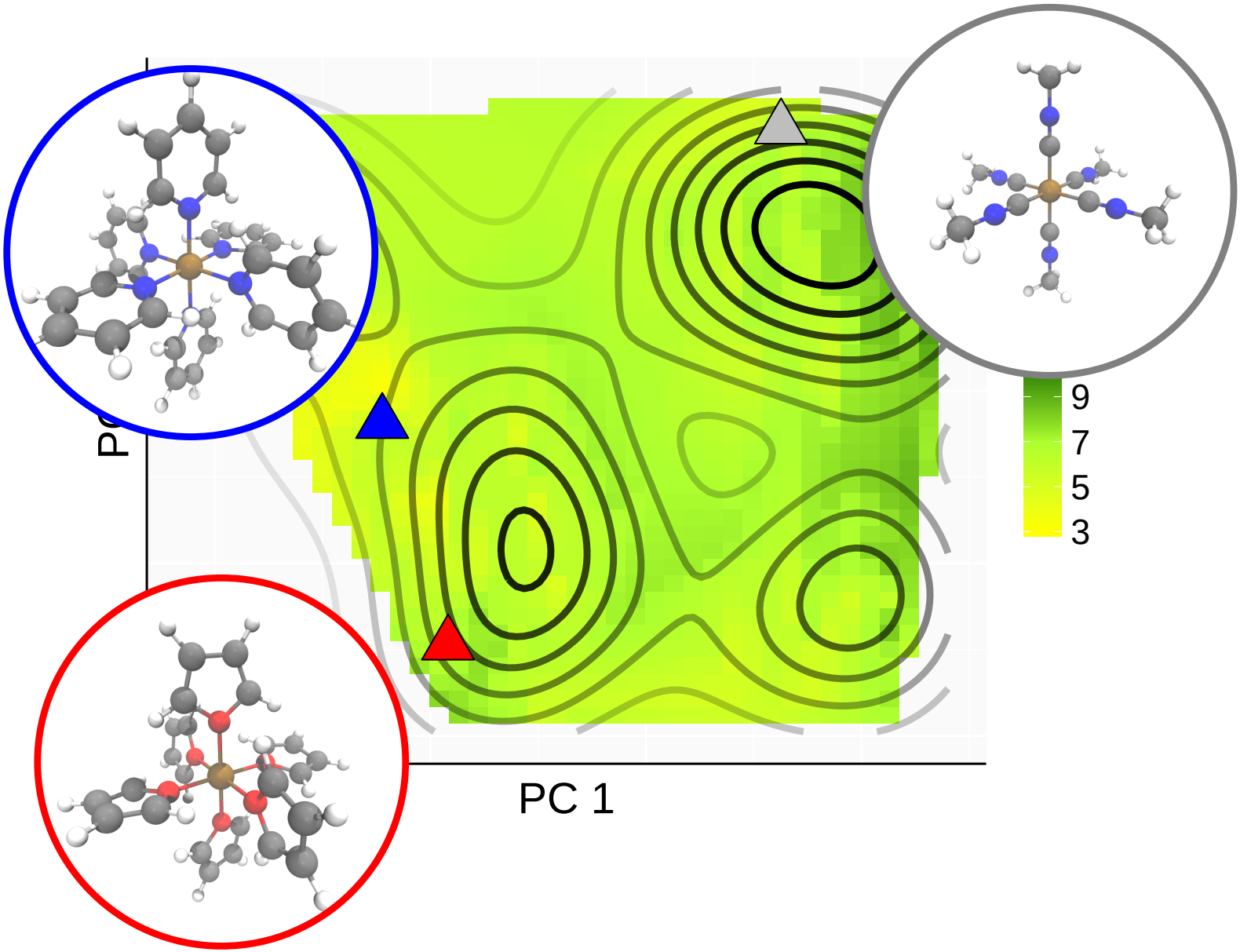

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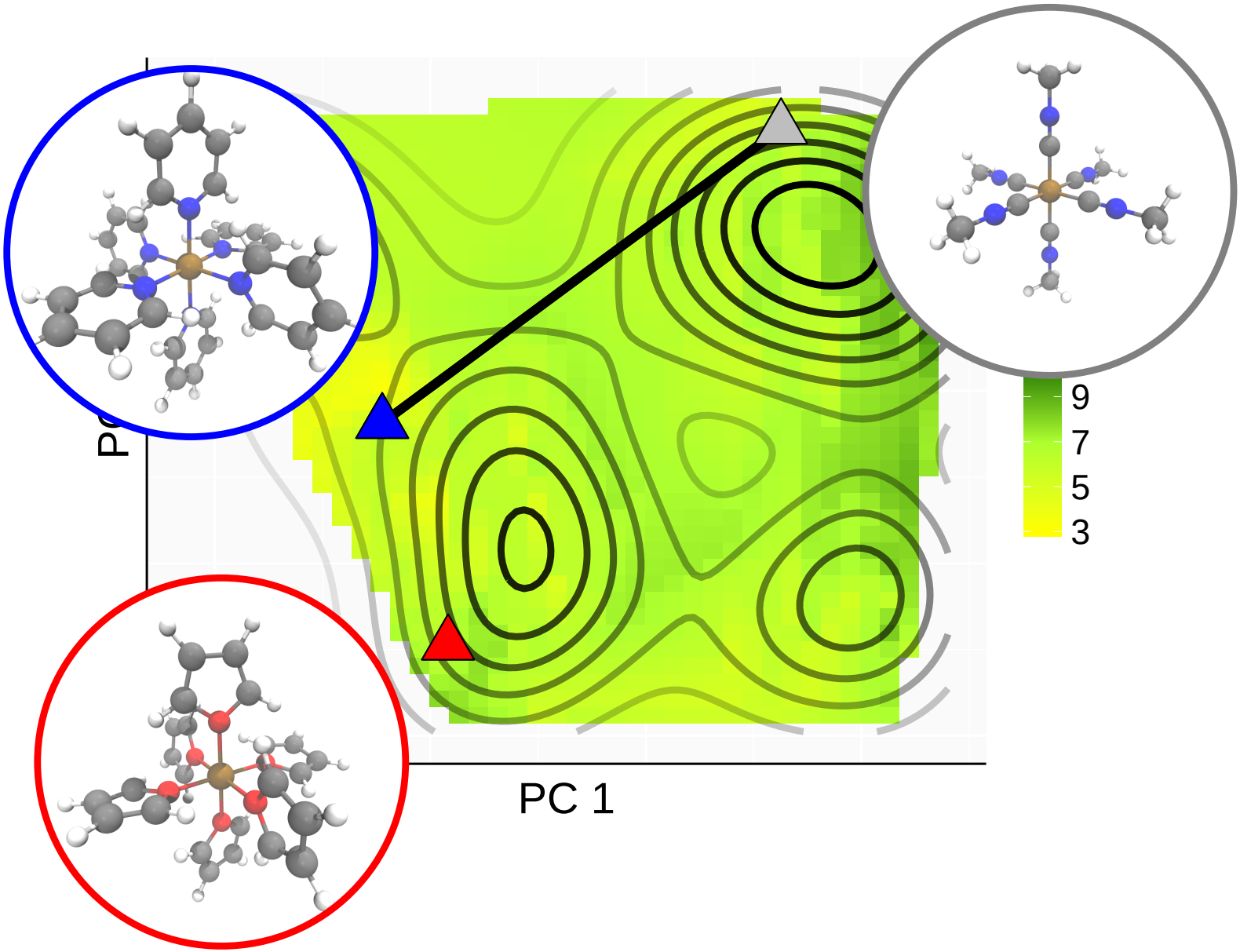

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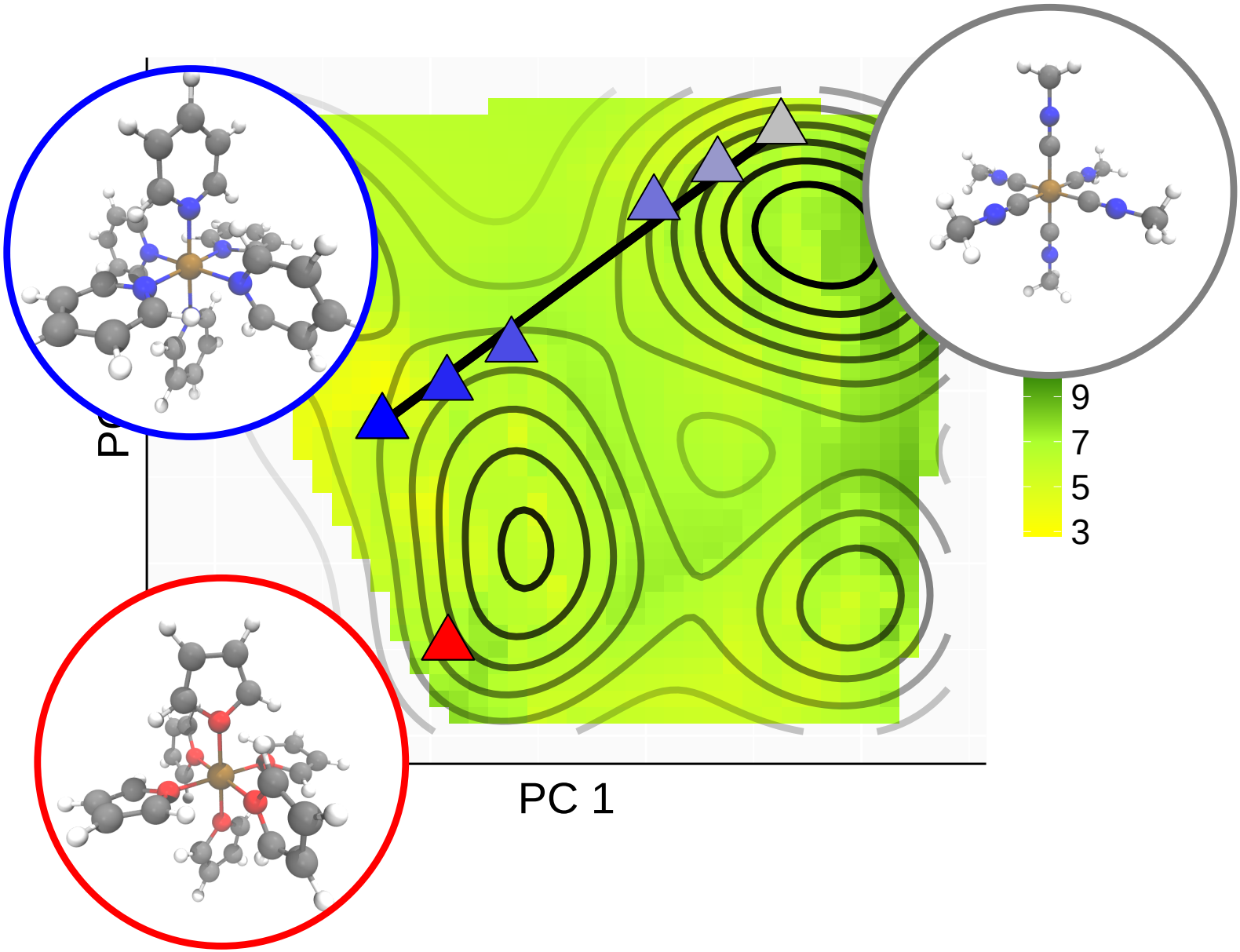

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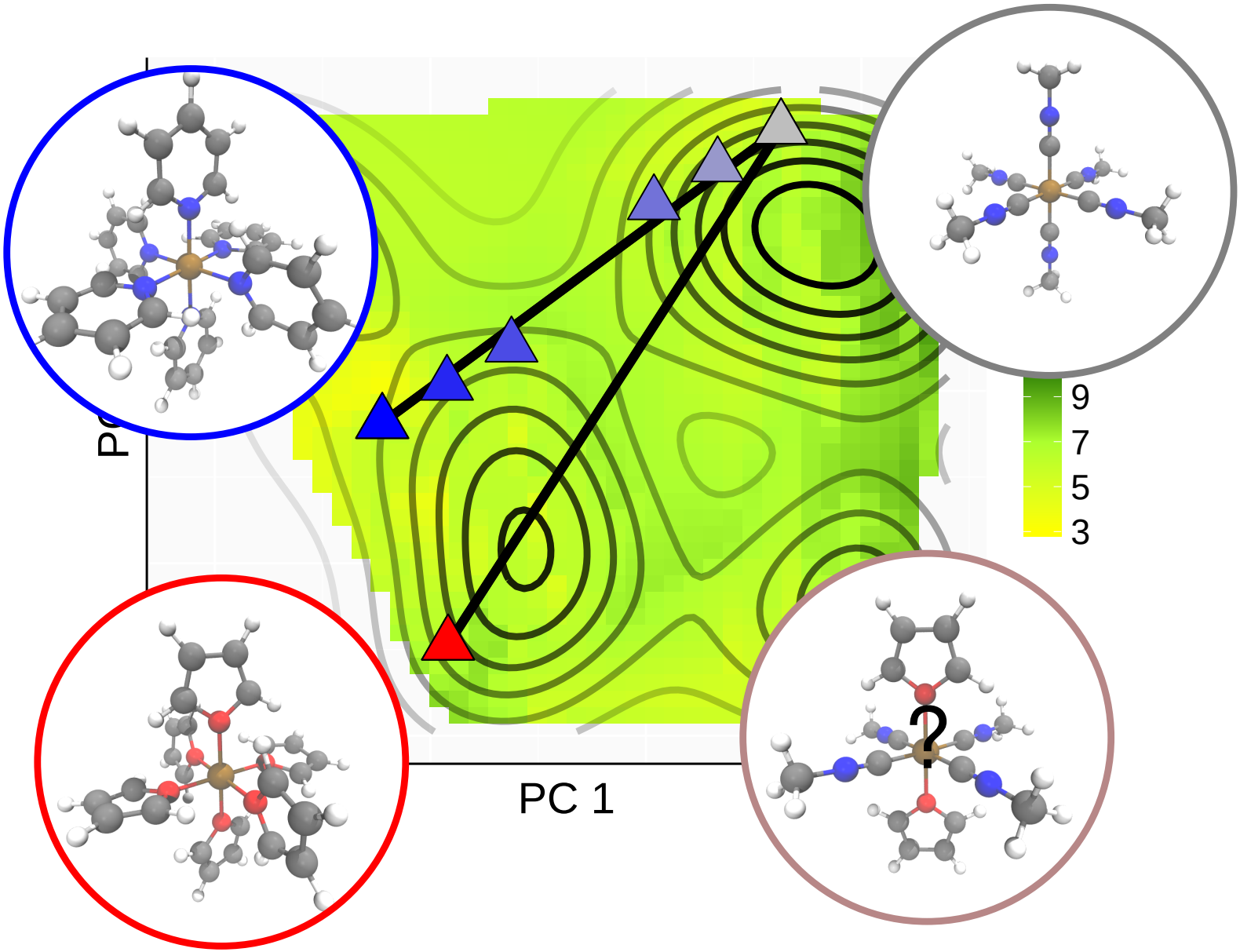

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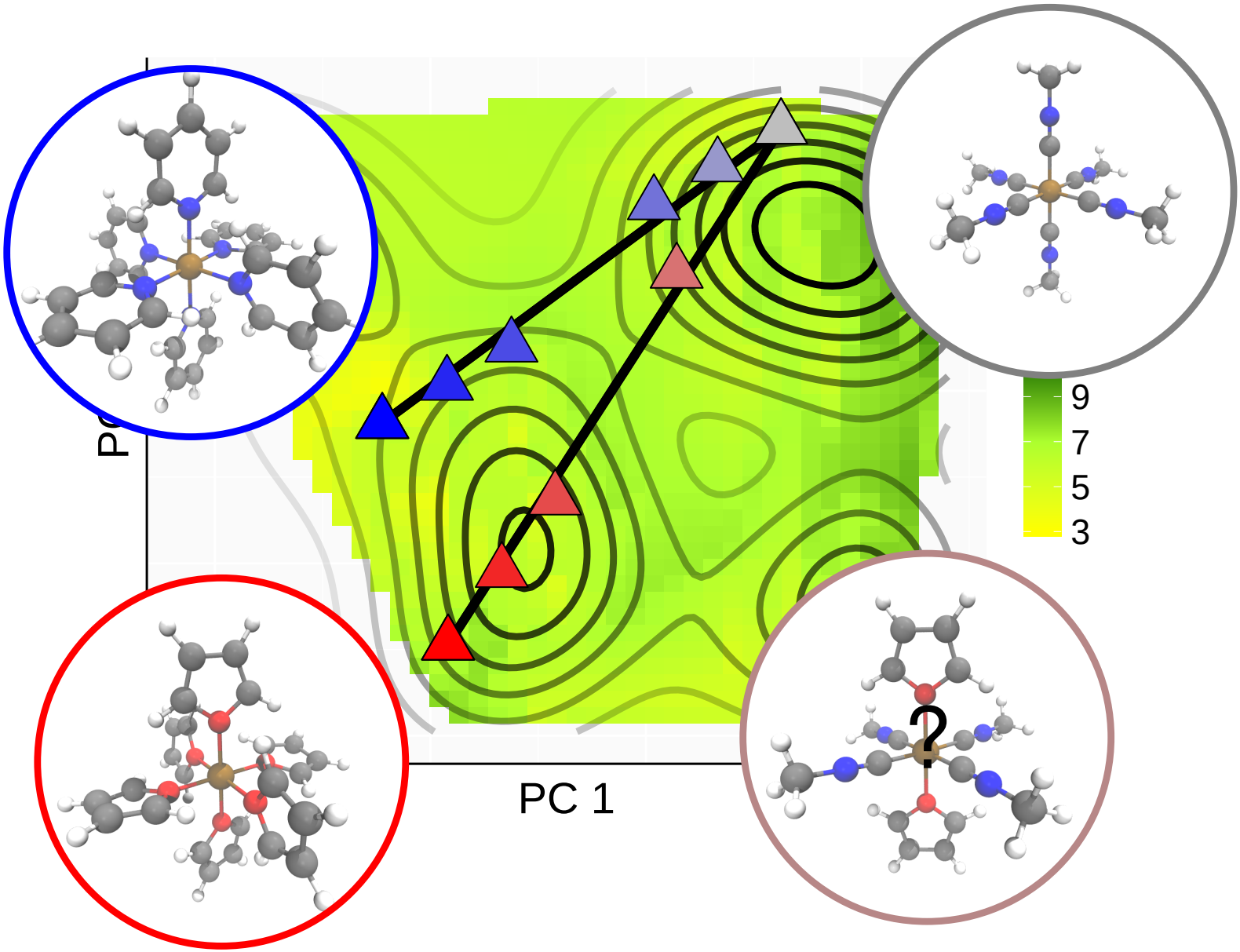

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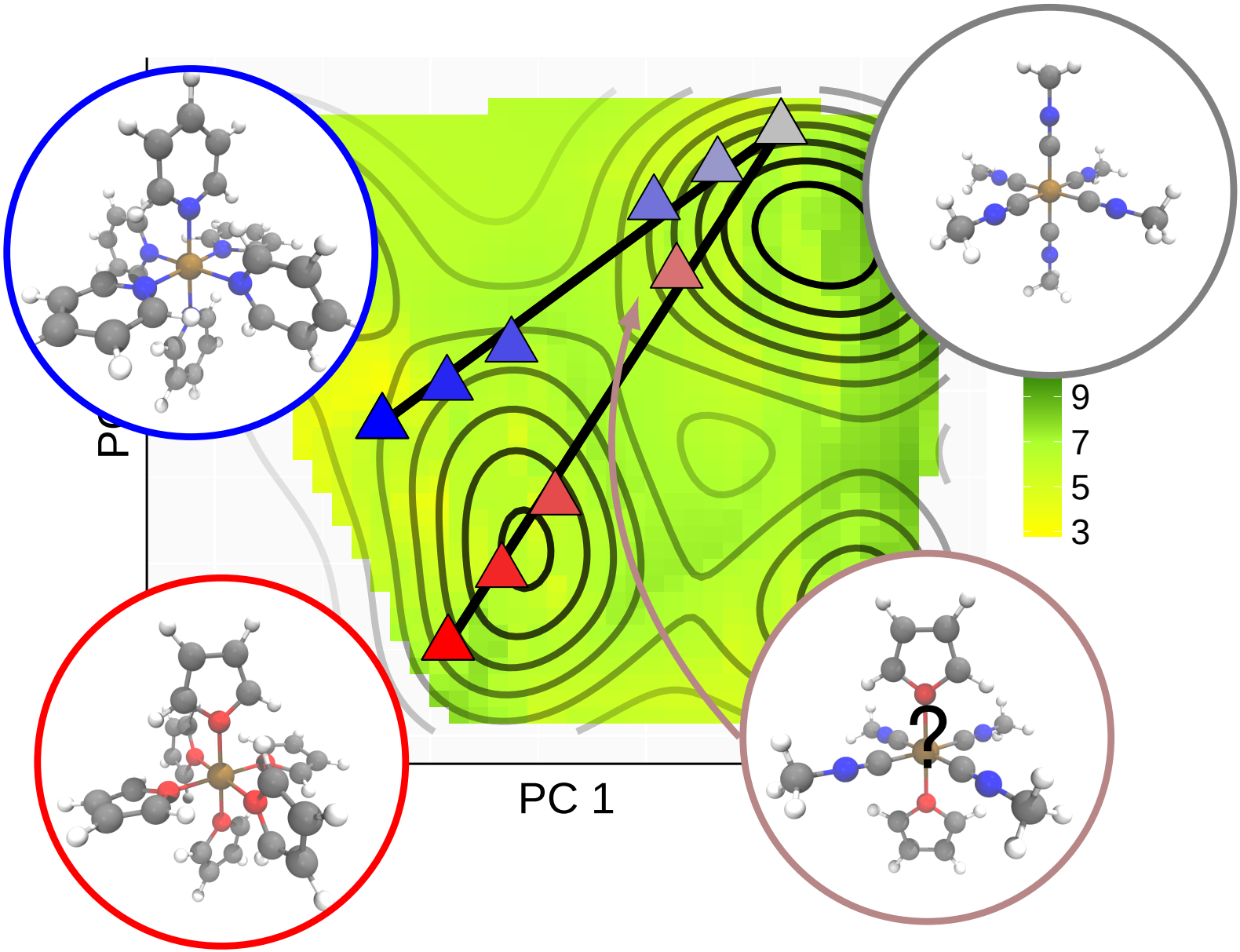

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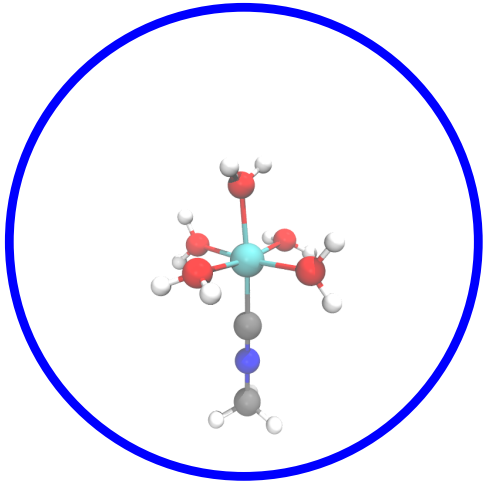

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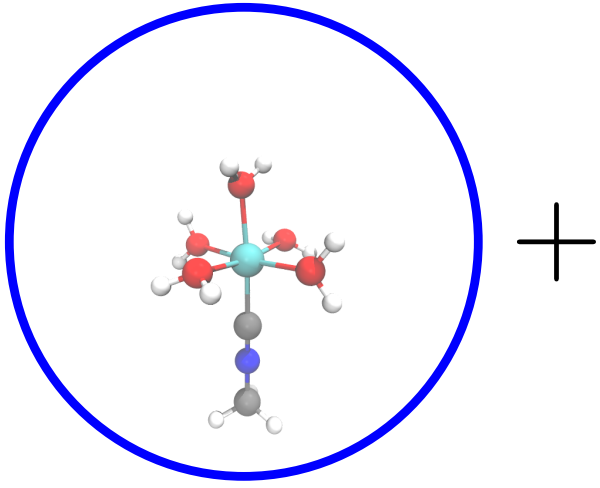

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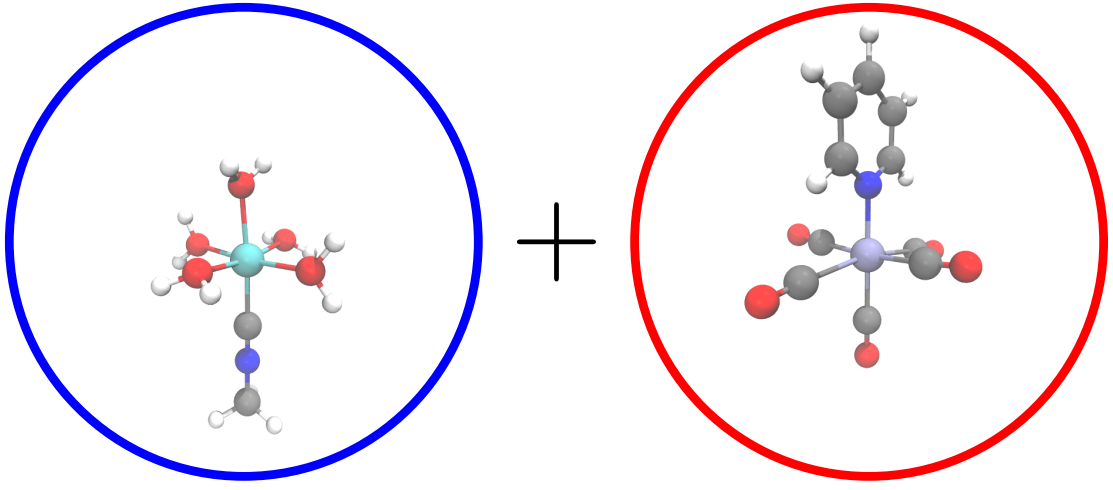

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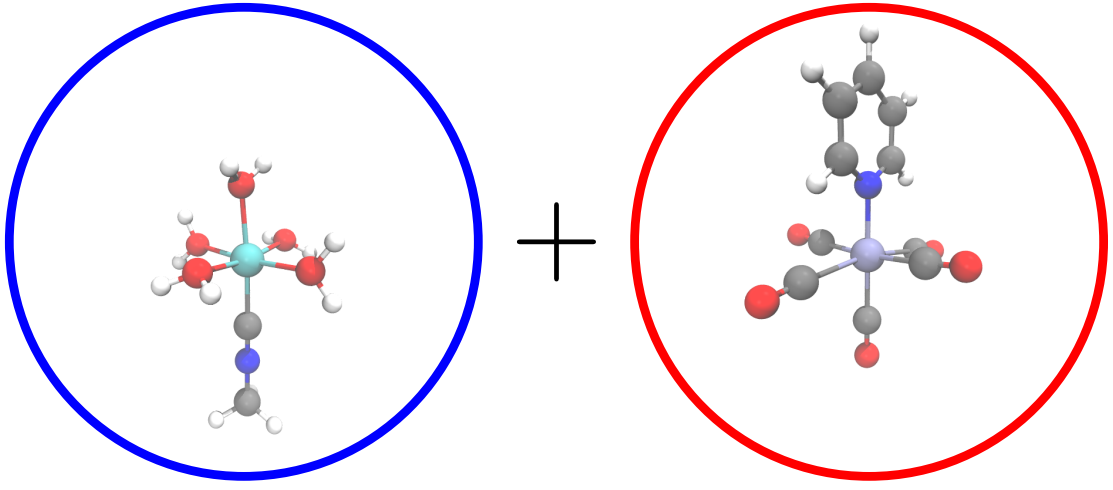

$$\frac{\quad + \quad}{2}$$

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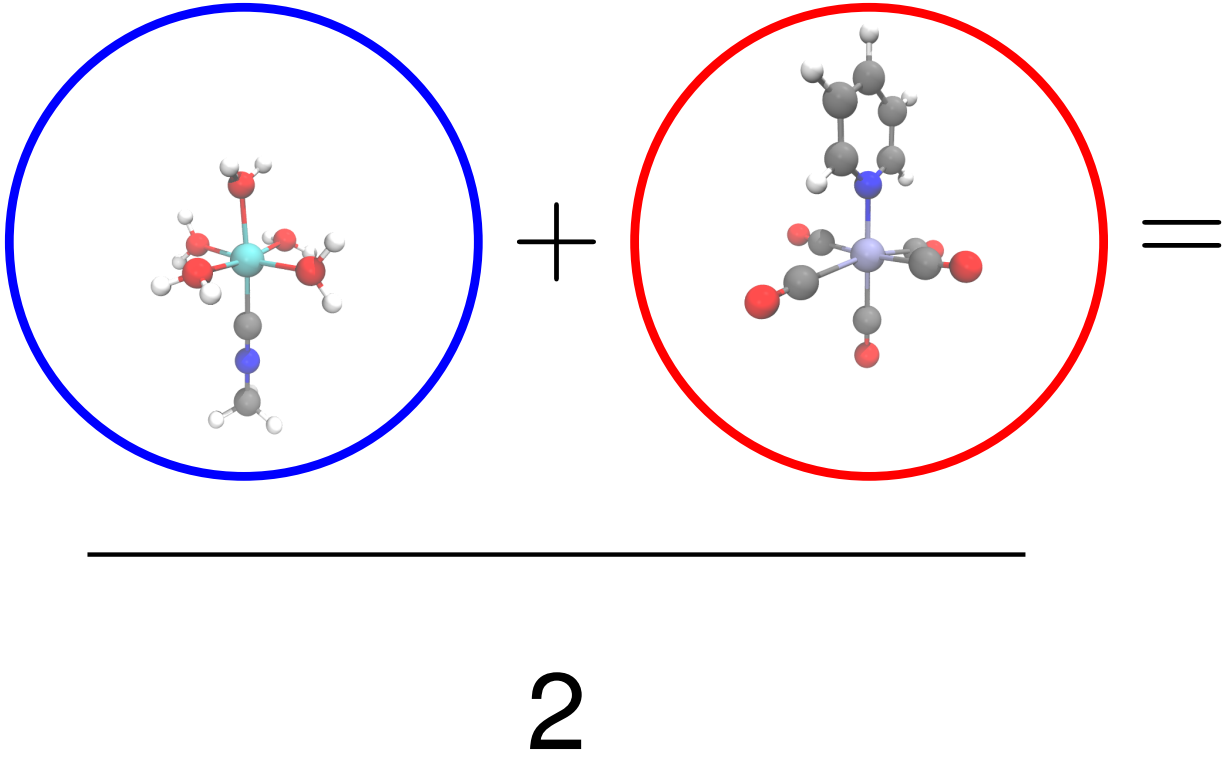

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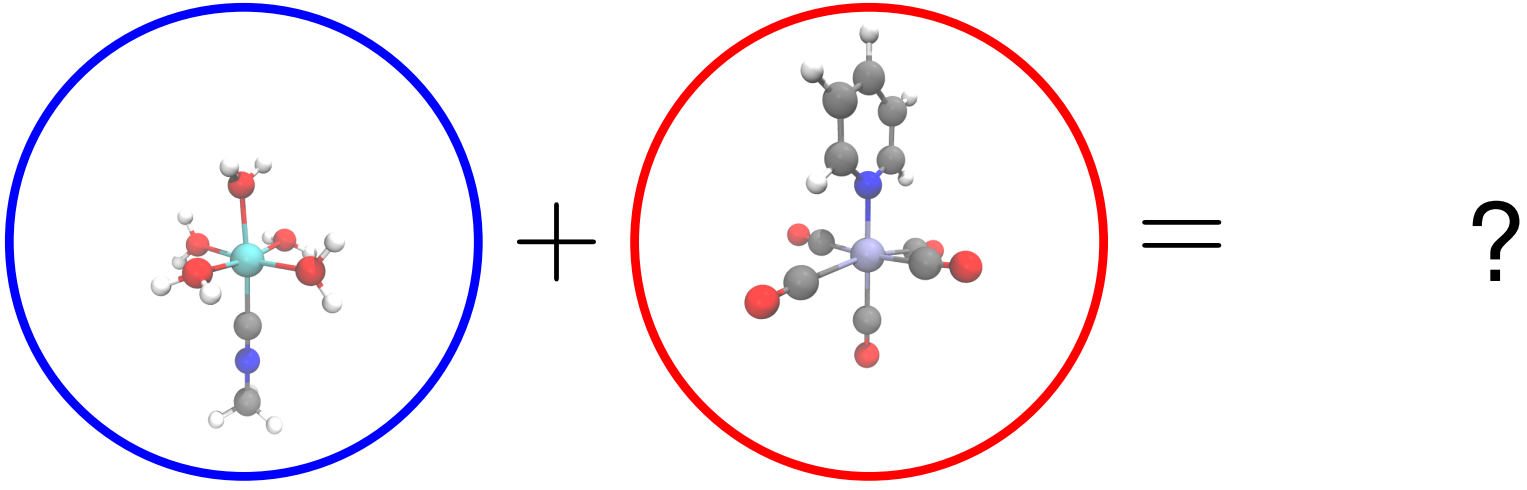

$$\frac{\quad + \quad}{2} = \; ?$$

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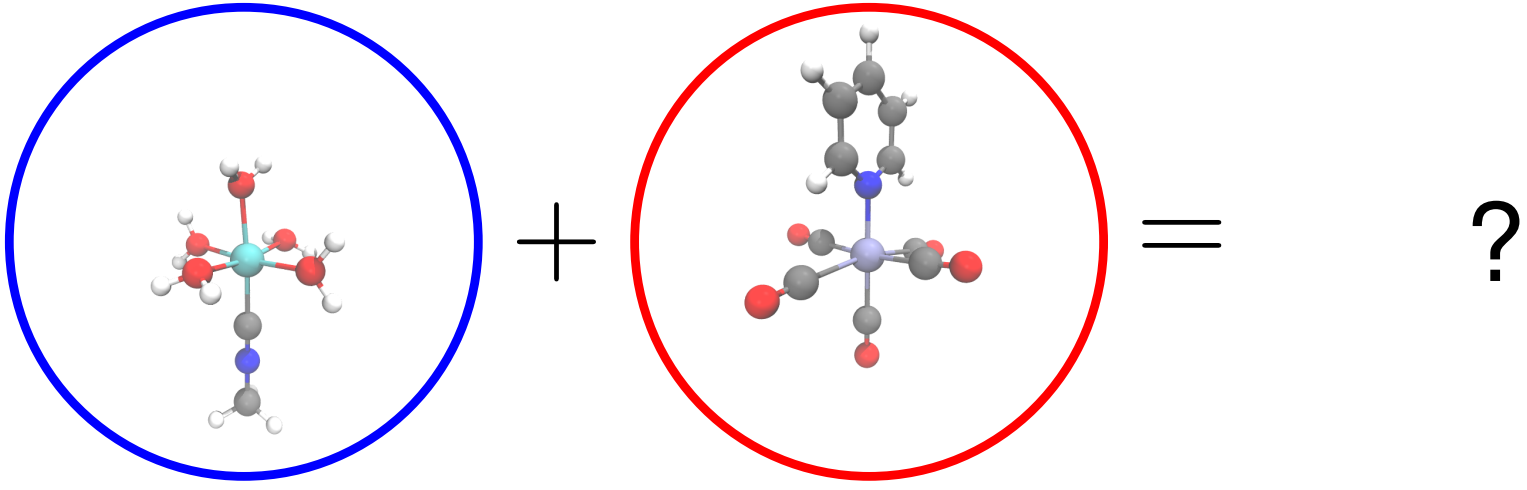

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Cr(II) $[H_2O]_5$ [misc] Co(II) $[CO]_5$ [pyr]

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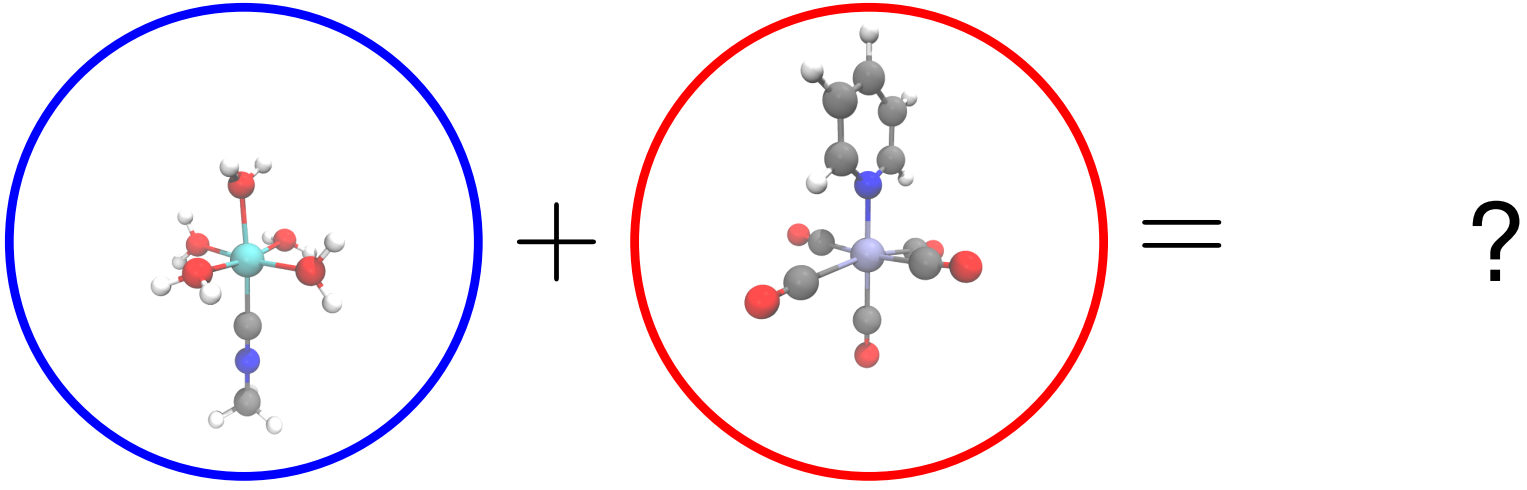

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$\mathrm{Cr(II)\,[H_2O]_5\,[misc]}$
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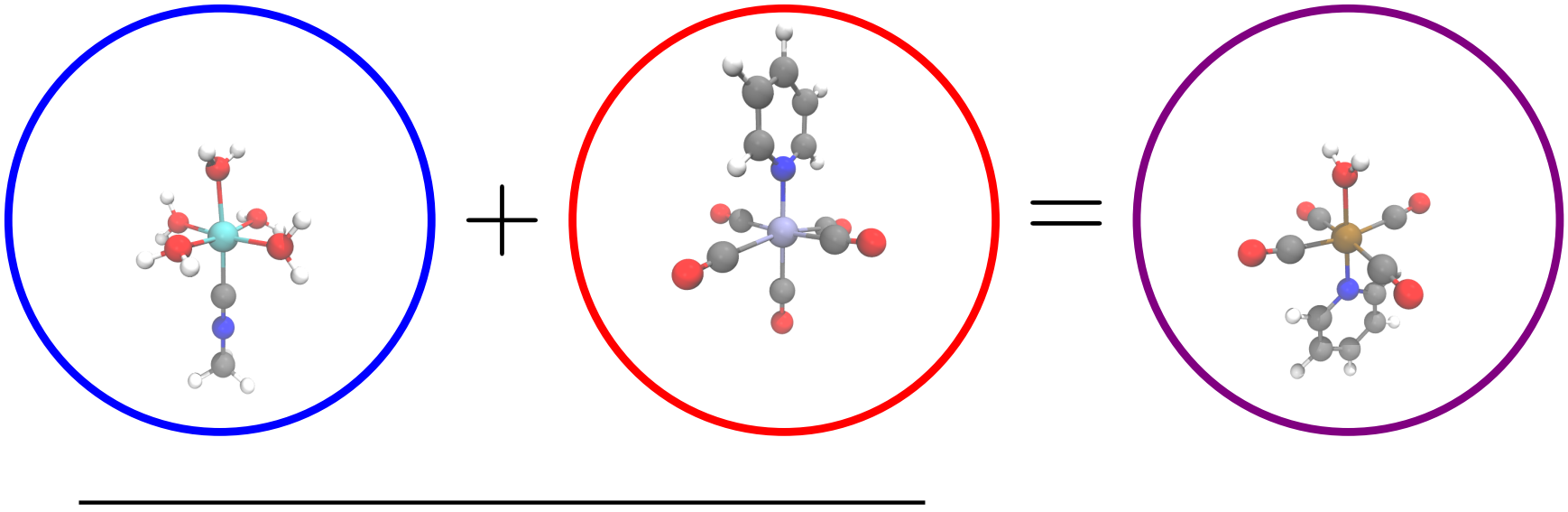

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$\mathrm{Fe(II)\,[CO]_4\,[pyr]\,[water]}$
$\Delta G = 7.8$ eV

Model transferability

Test-set performance is not necessarily a good metric for general transferability[2]:

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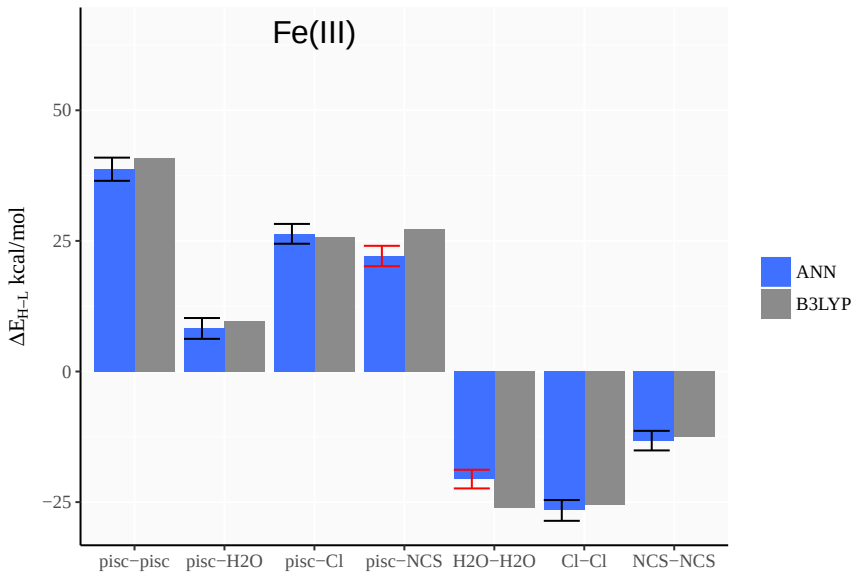

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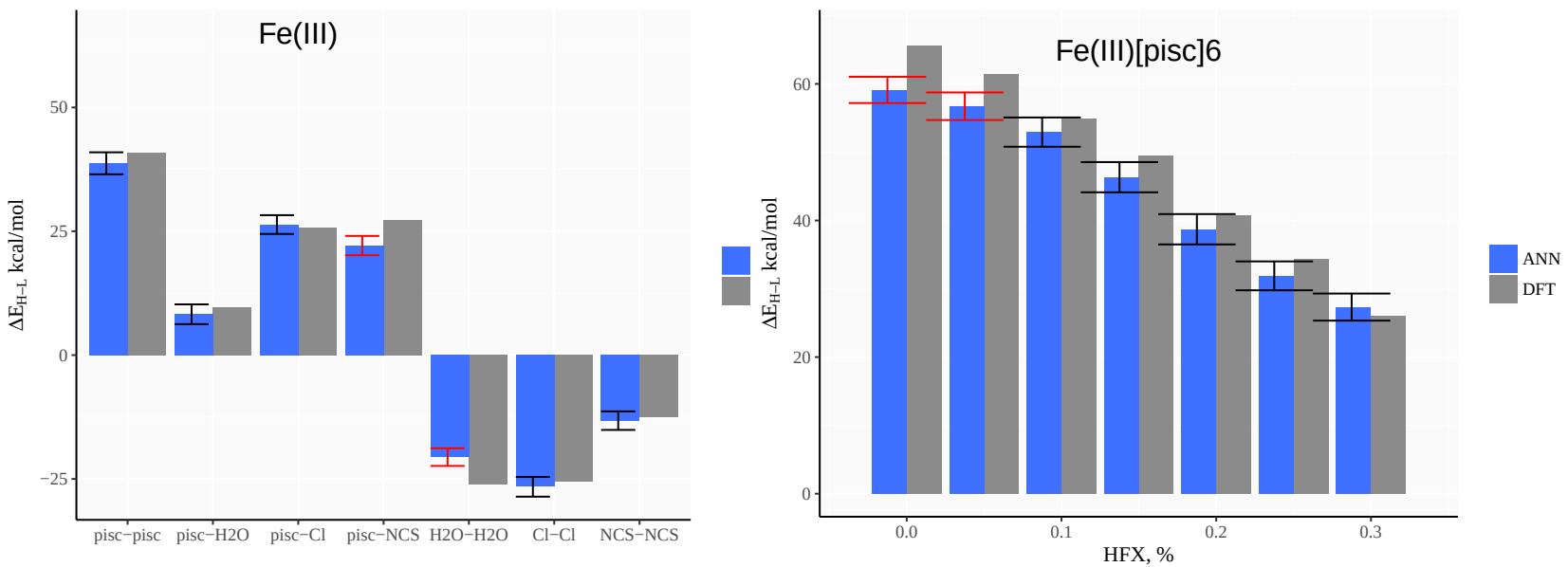

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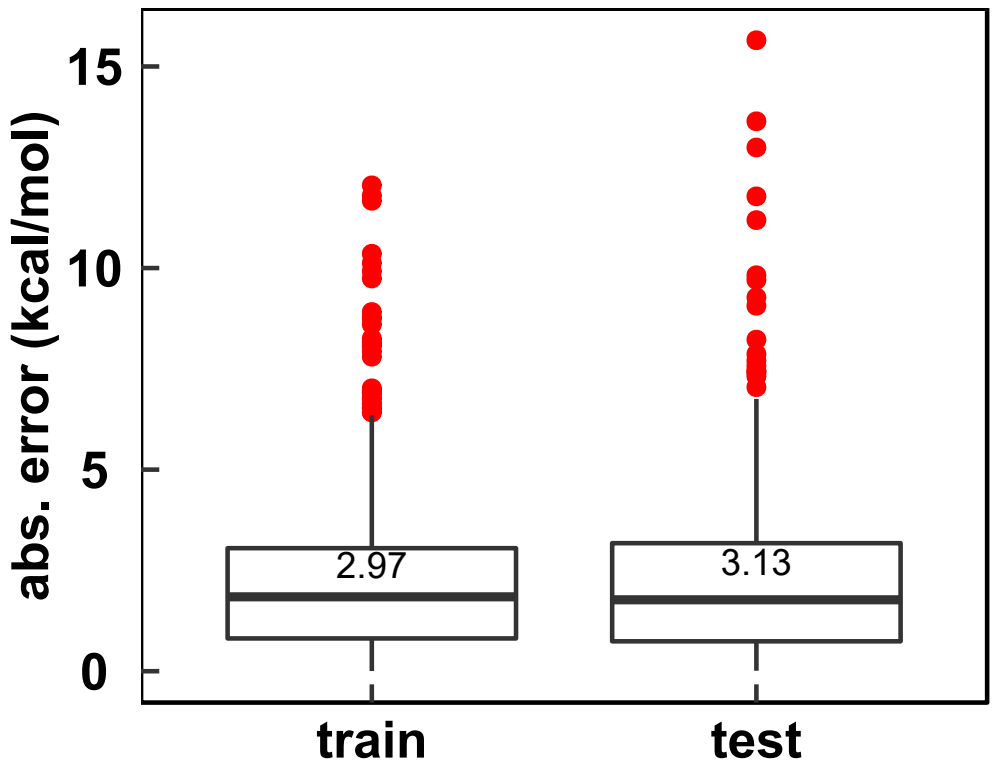

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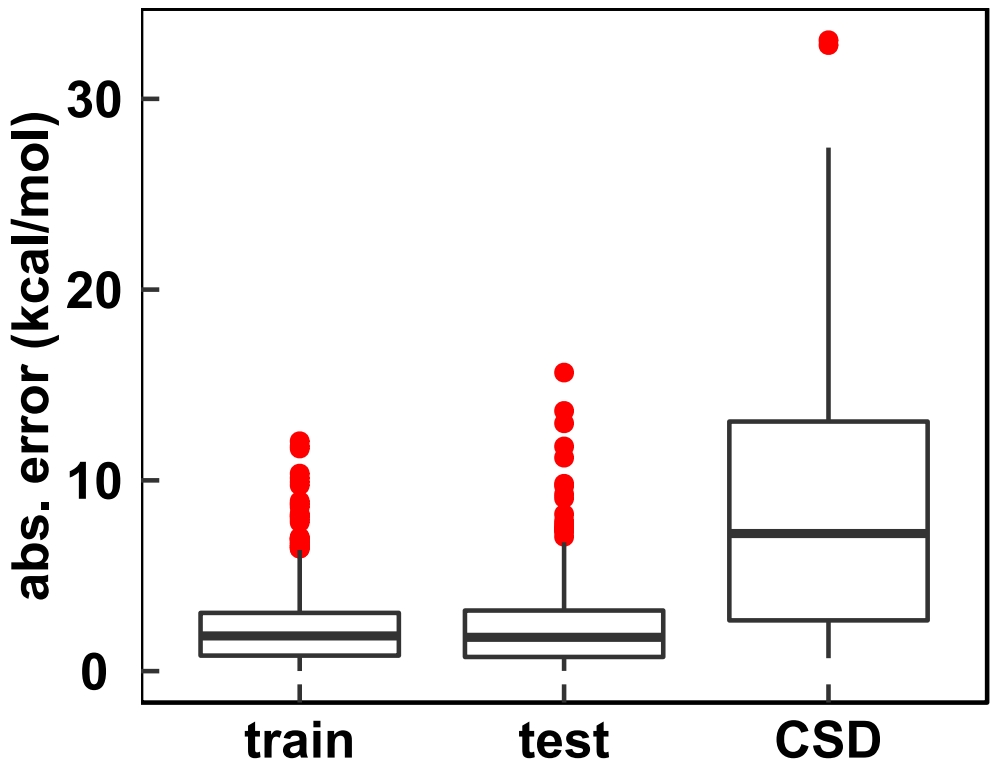

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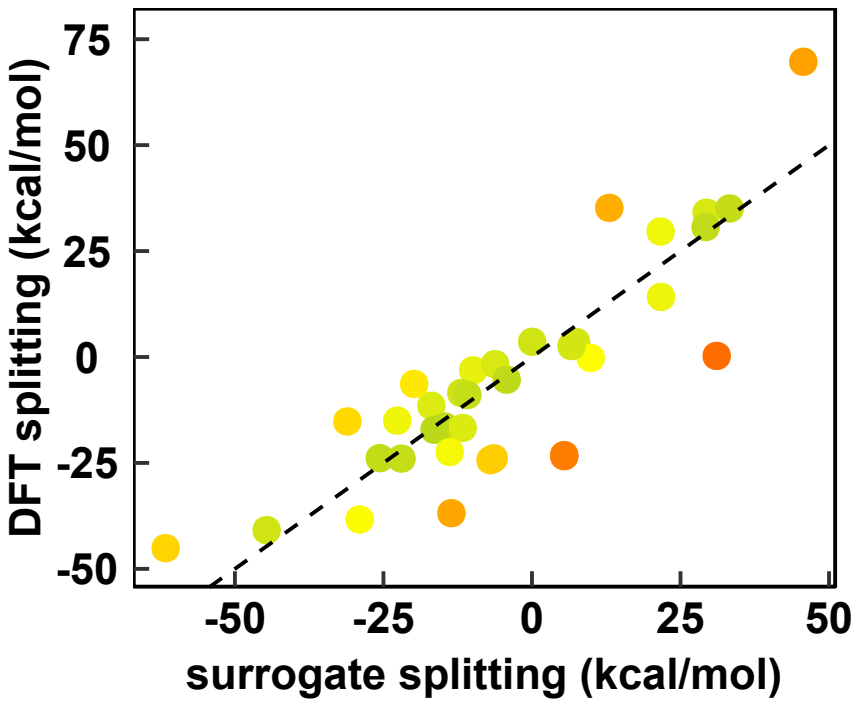

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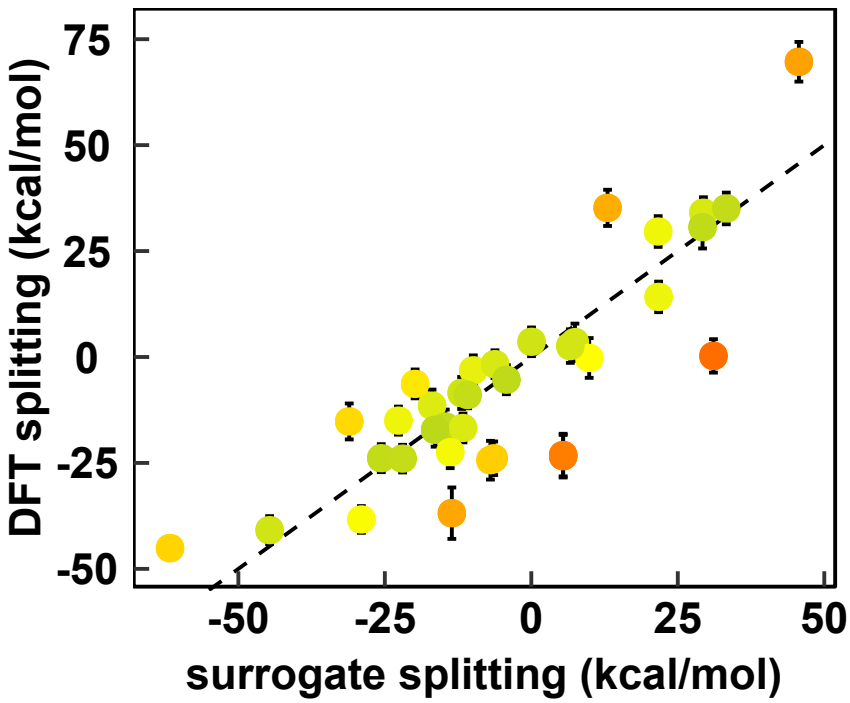

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$$\mathrm{var}\left(y^* \middle| x^*\right) \approx \frac{1}{J}\sum_j \hat{y}_j^T \hat{y}_j + \tau^{-1}$$

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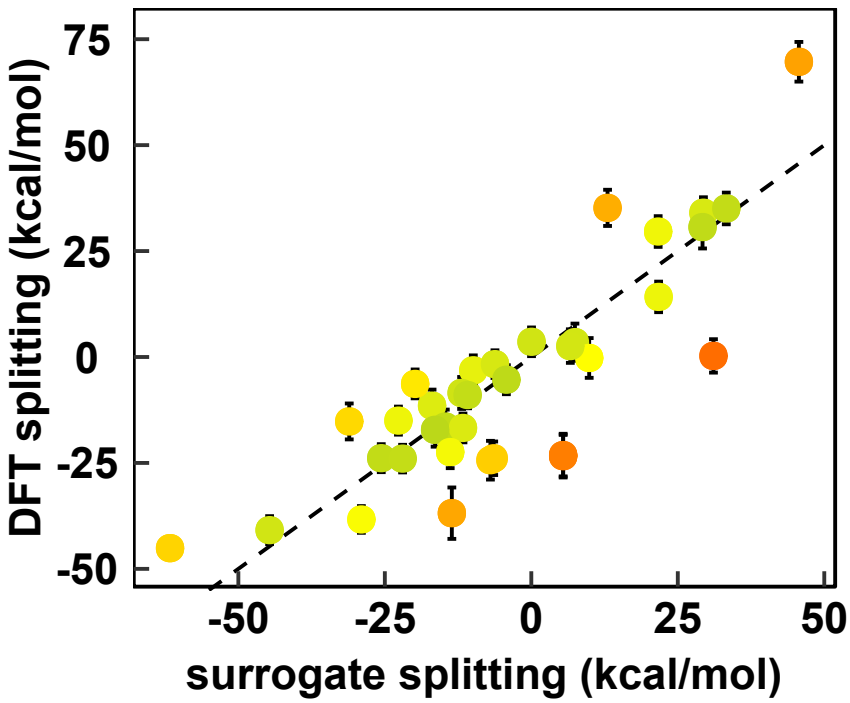

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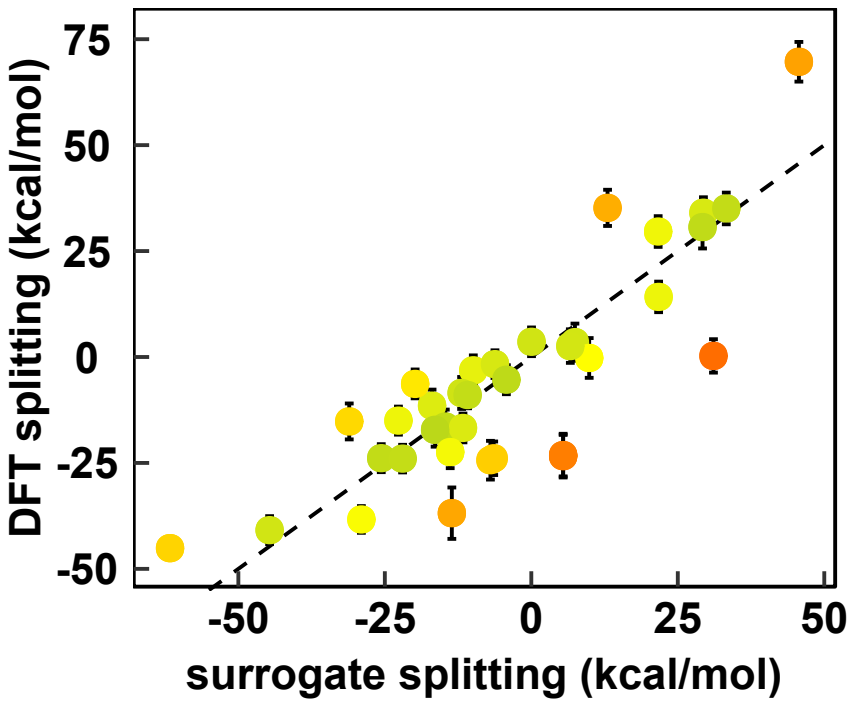

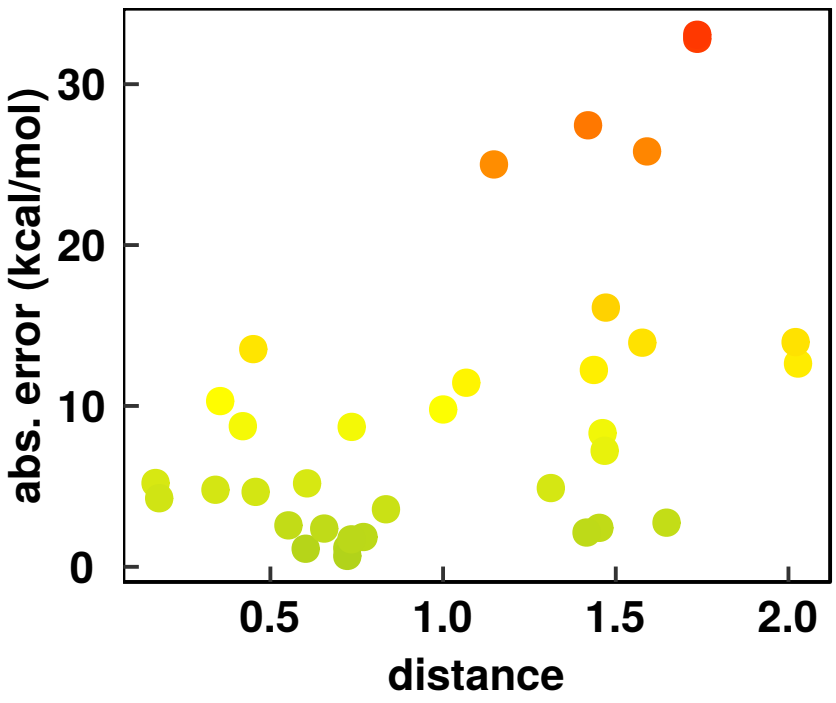

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Can we use the ANN model to find new spin-crossover materials, i.e. $\Delta E_{H-L} = 0$?

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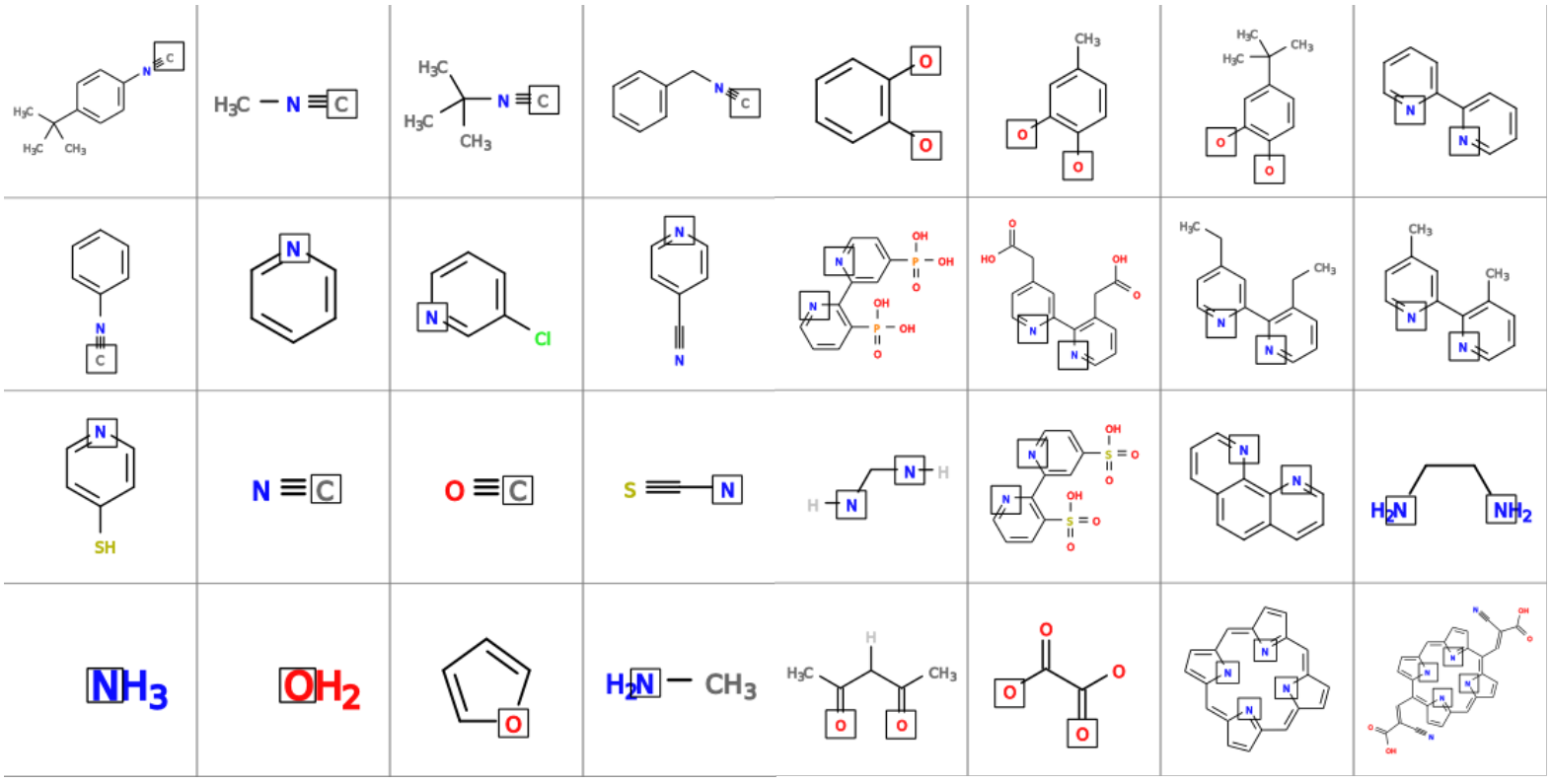
Can we use the ANN model to find new spin-crossover materials, i.e. $\Delta E_{H-L} = 0$? Define a space of 32 ligands, 5 metals and with $\sim$ 5600 possible elements with forced axial/equatorial symmetry[3]:



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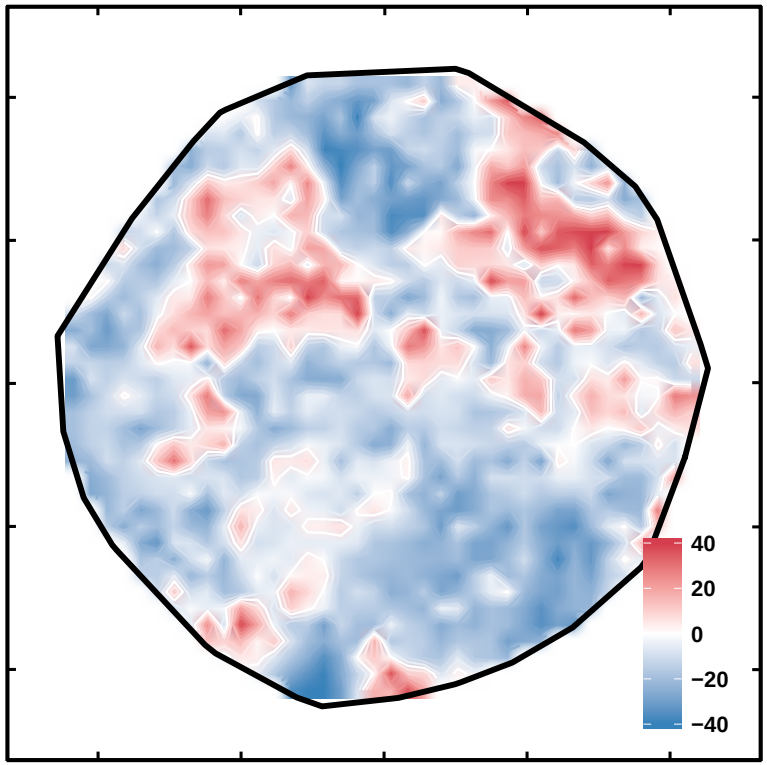

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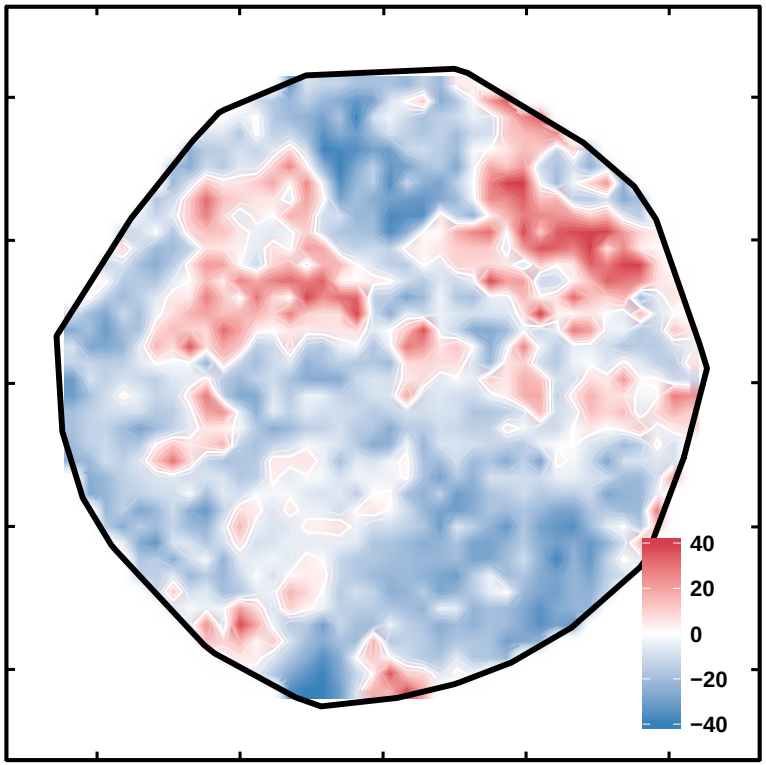

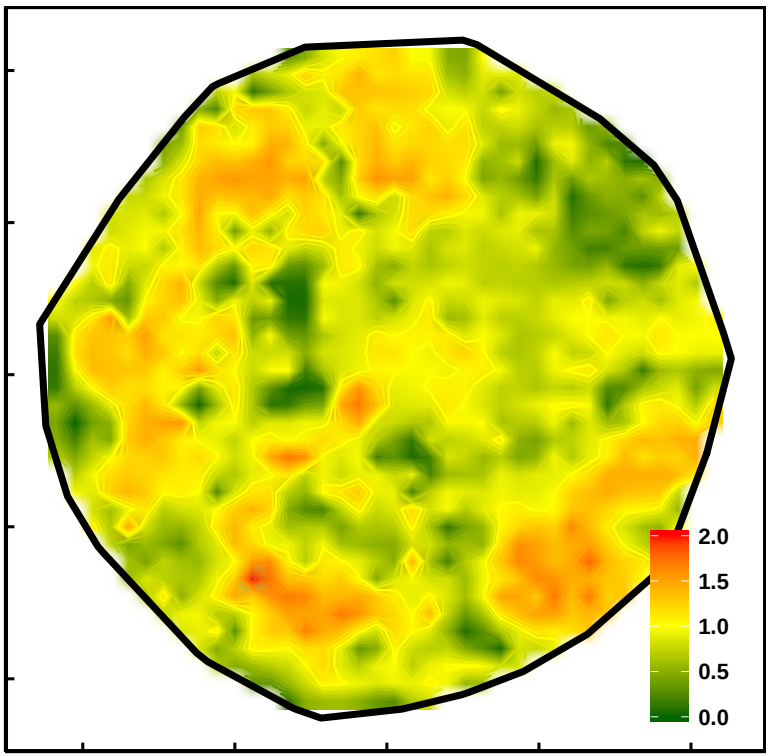

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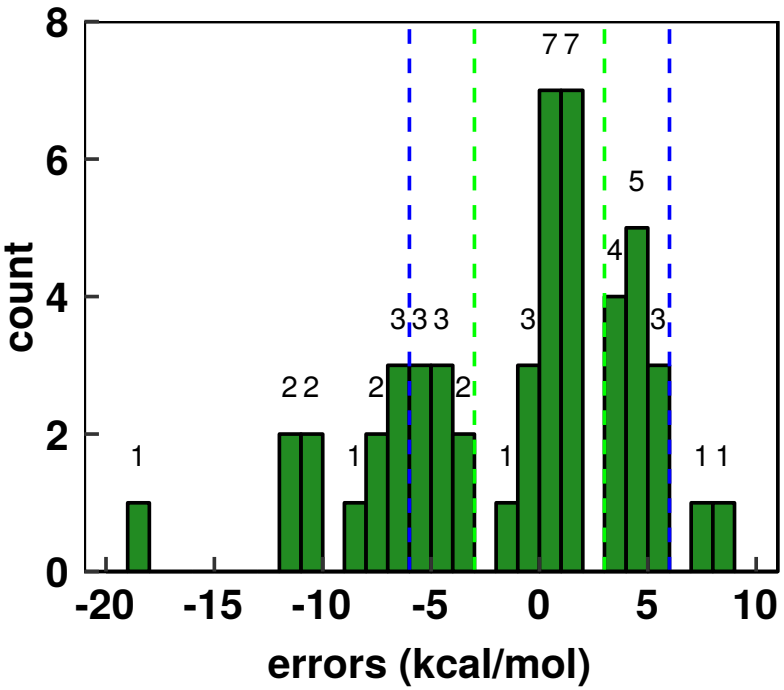

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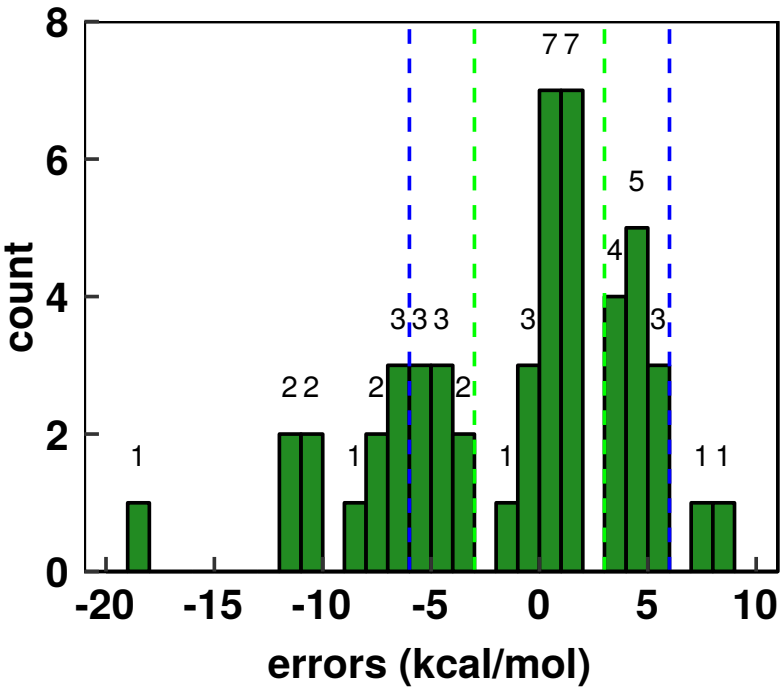

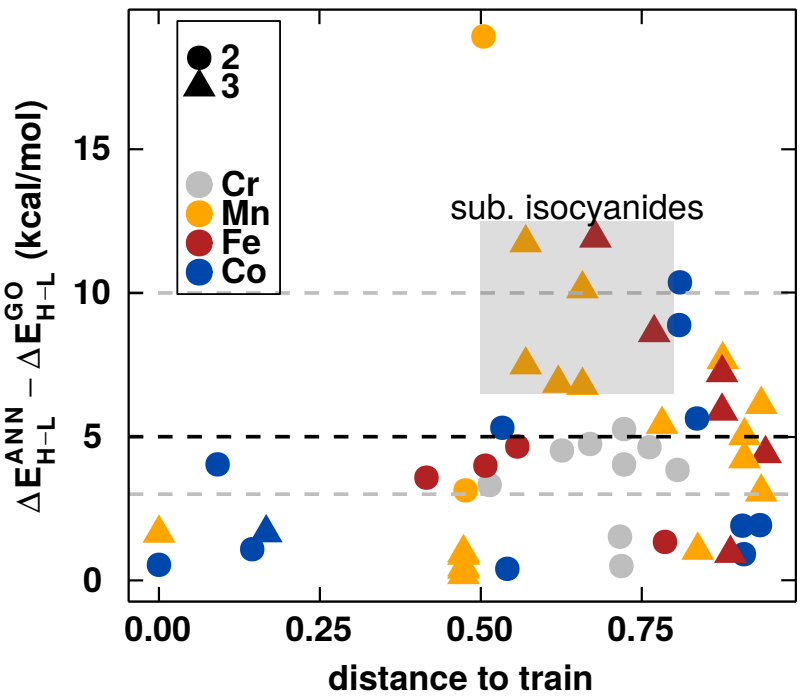

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Conclusions

- choice of molecular representation is important
- different properties depend non-equally on features
- feature-space geometry can provide insight into model reliability
- imbuing ‘chemical intuition’ to descriptor construction can drastically improve learning
- conversely, feature selection can contribute to understanding systems

Acknowledgments

Thanks to the Kulik group and funding partners: