Mapping transition metal chemical space for machine learning models

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2017 AIChE Annual Meeting
Minneapolis, MN

11.01.17

Data-driven molecular design

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

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Gomez-Bombarelli, R. *et al.*. *Nat. Mater.*, 15(10):1120-1127, 2016.

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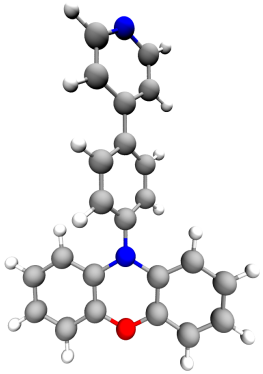

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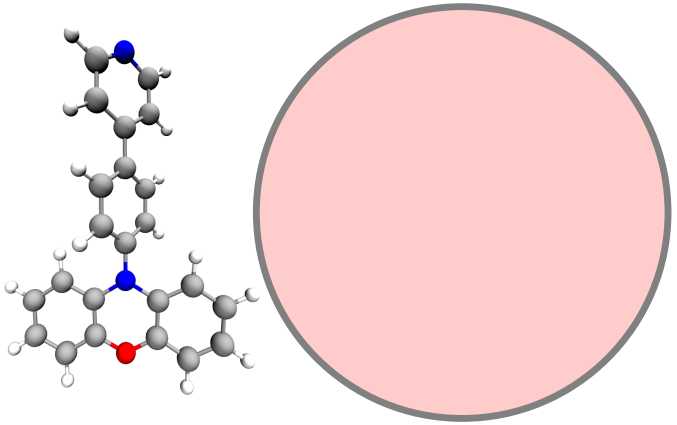

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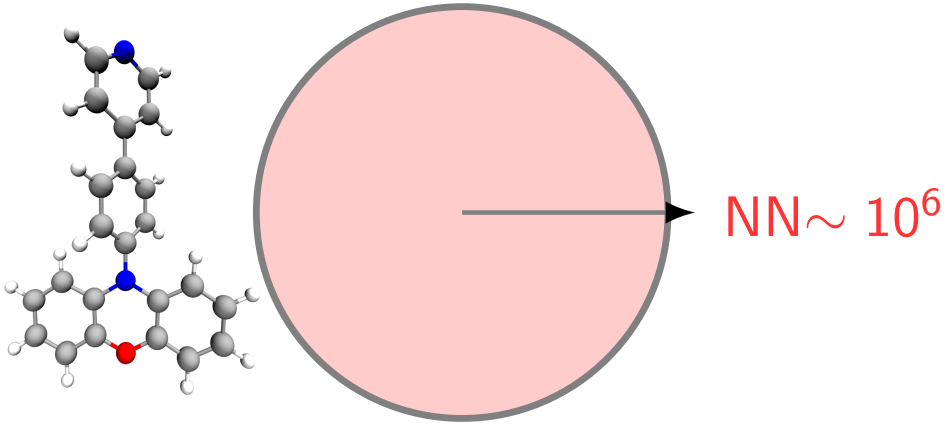

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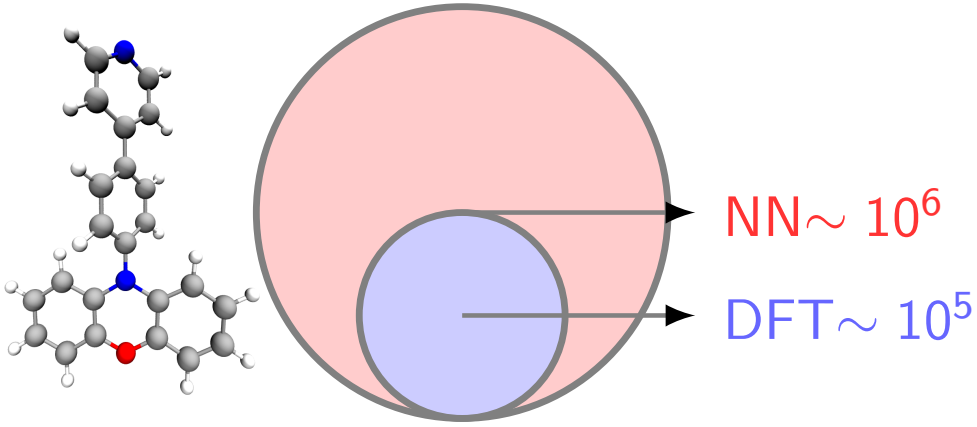

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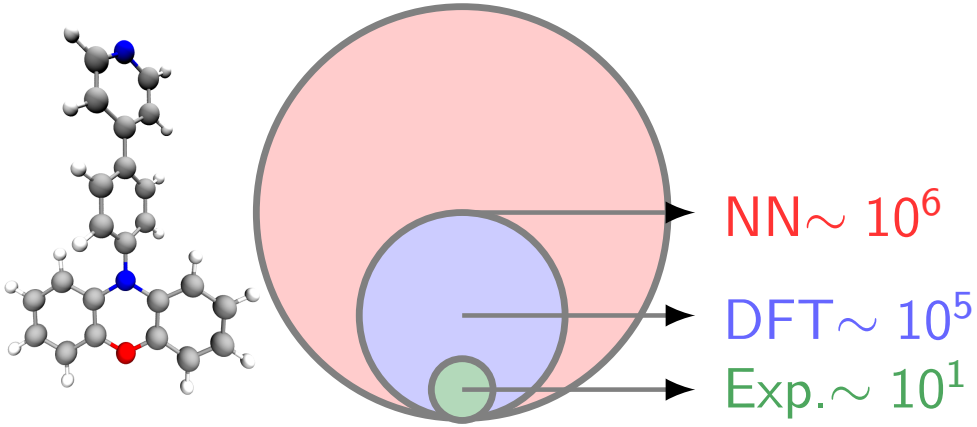

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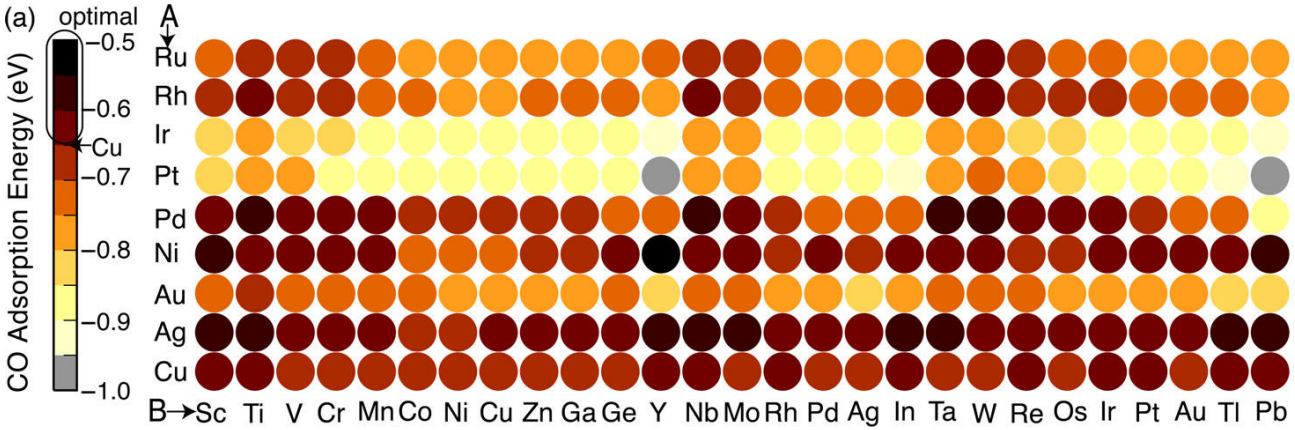

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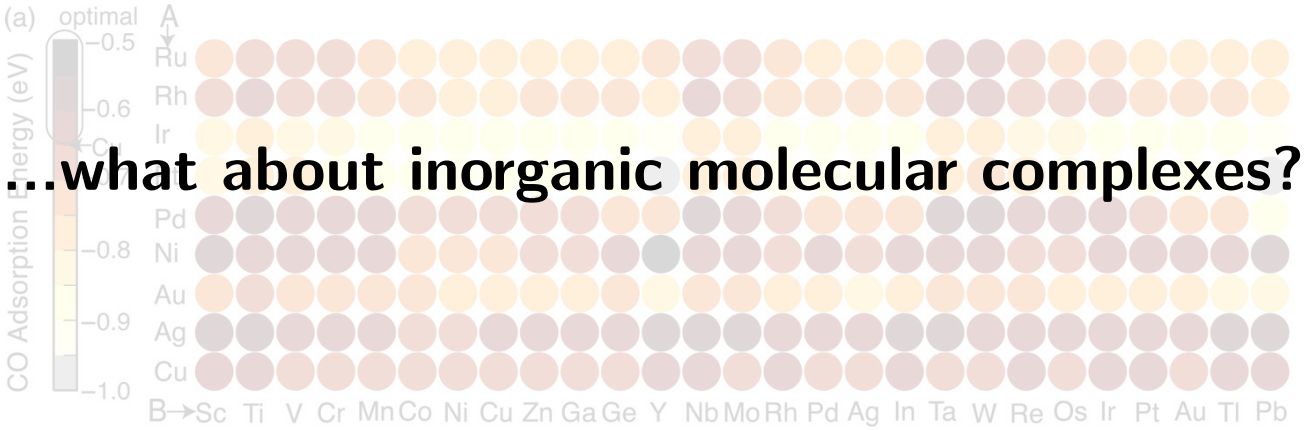

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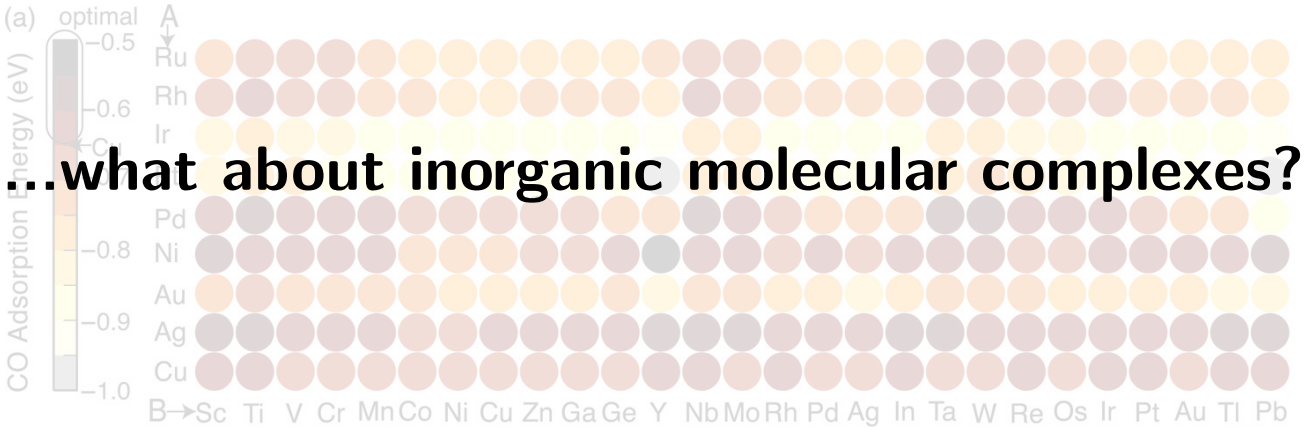

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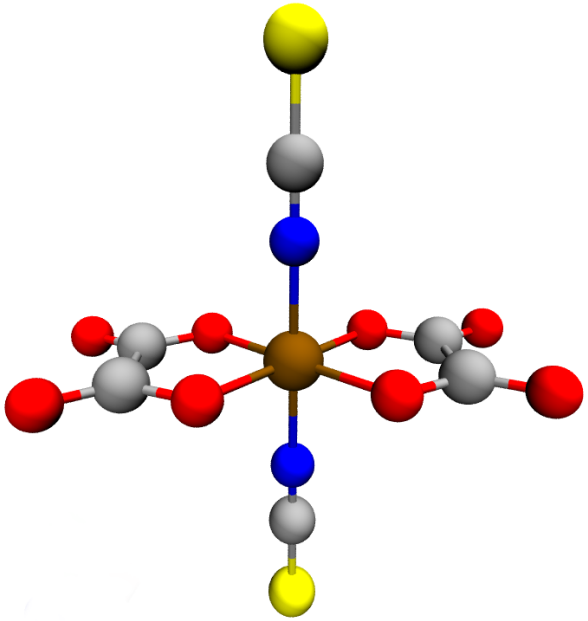

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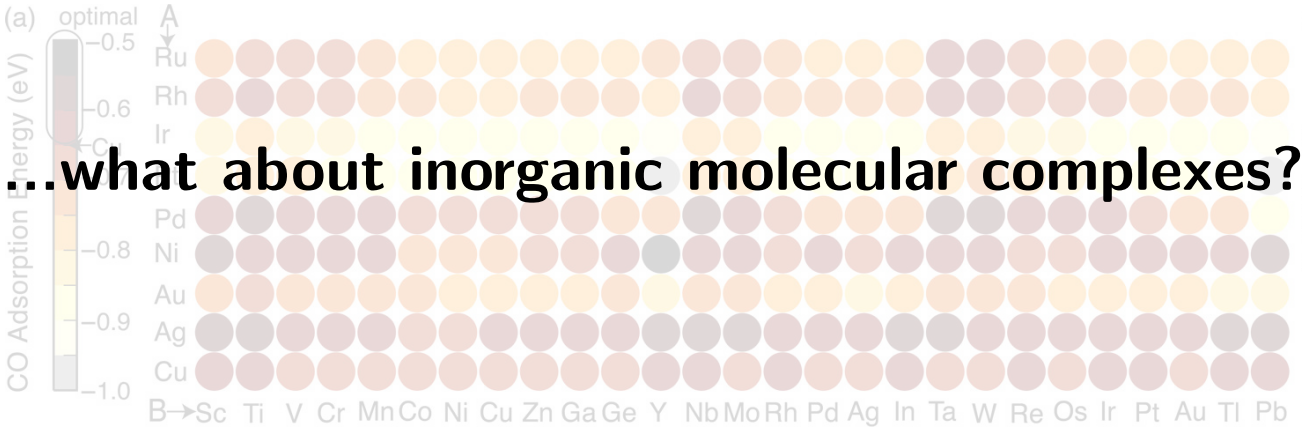

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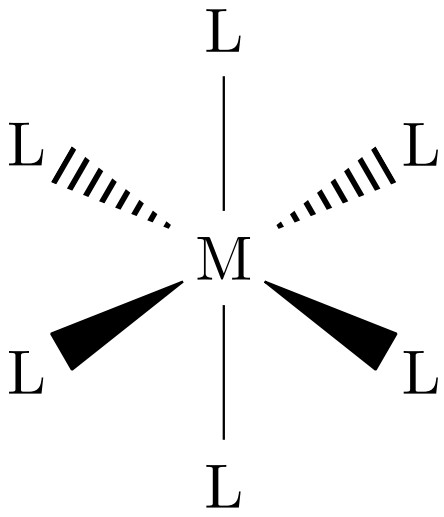

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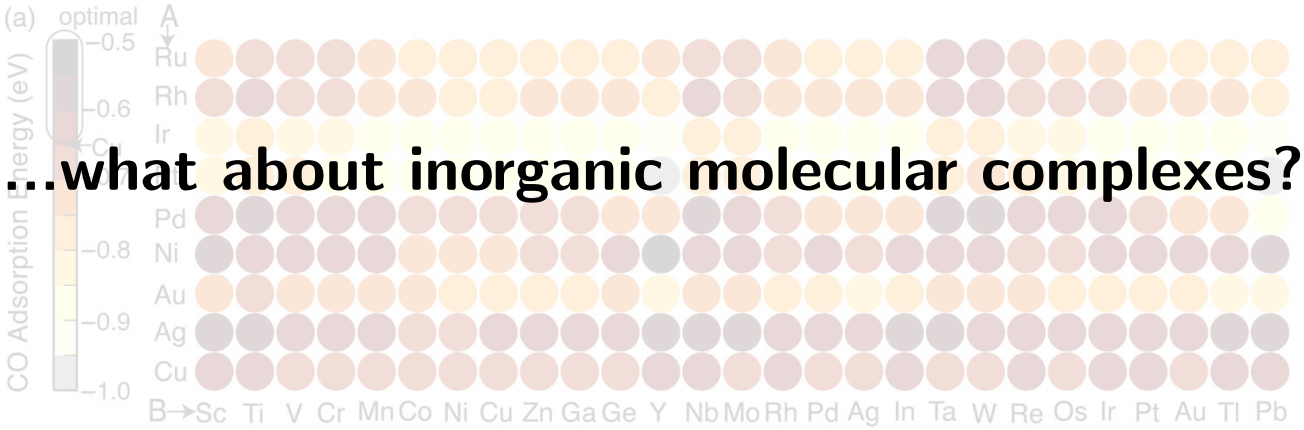

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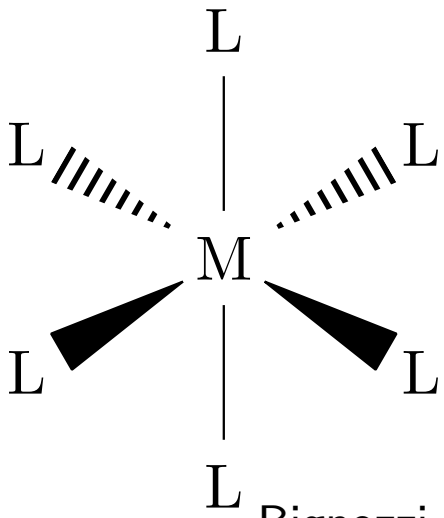

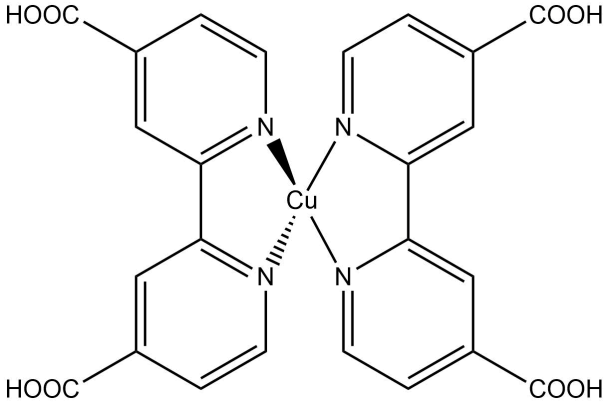

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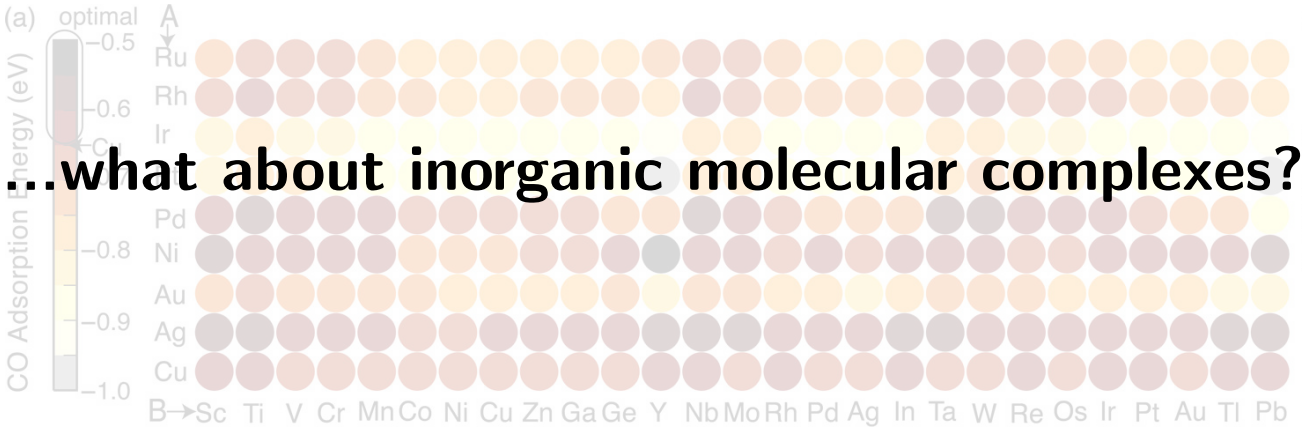

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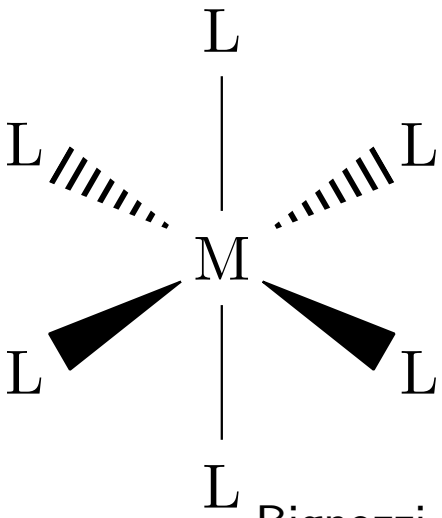

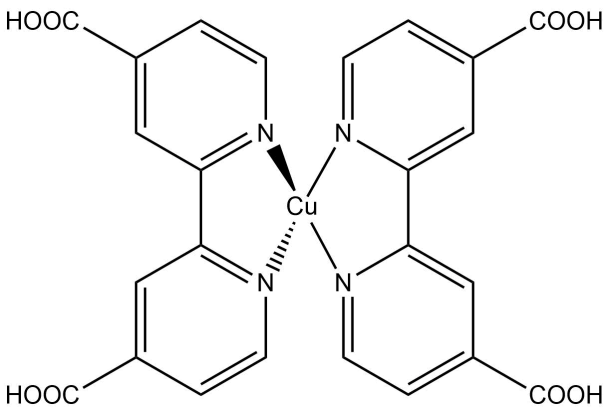

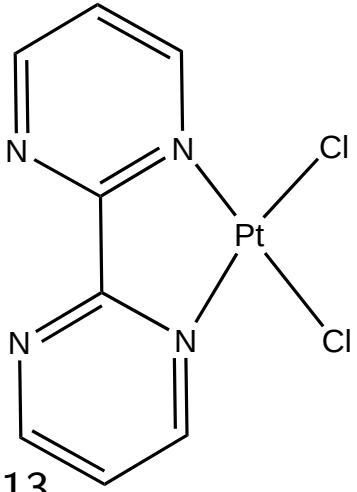

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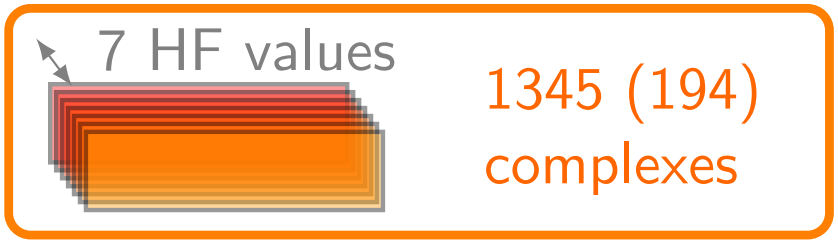

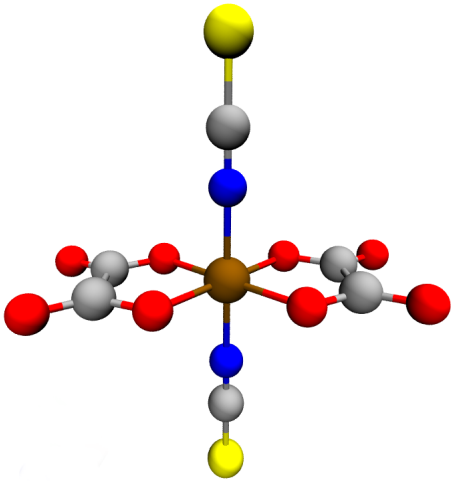

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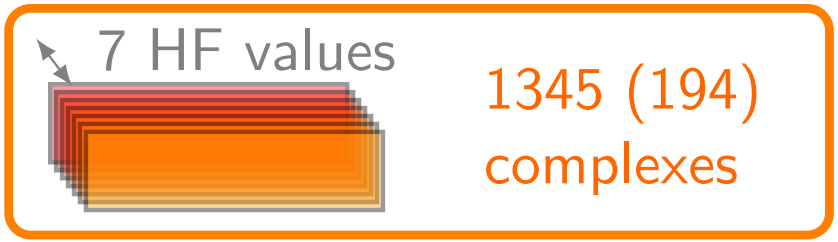

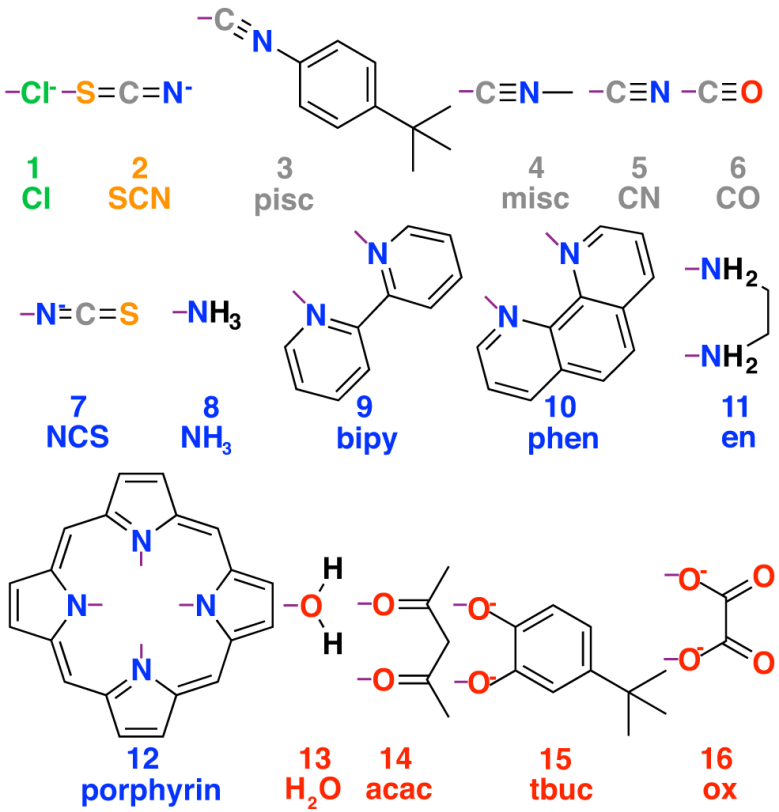

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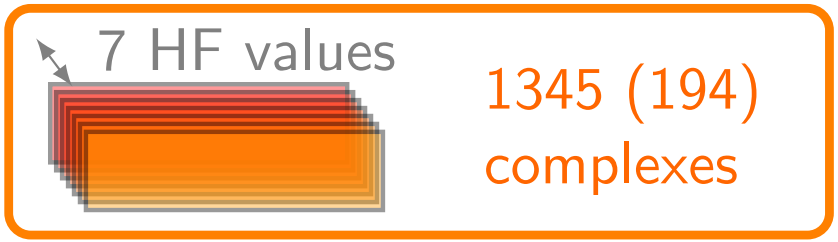

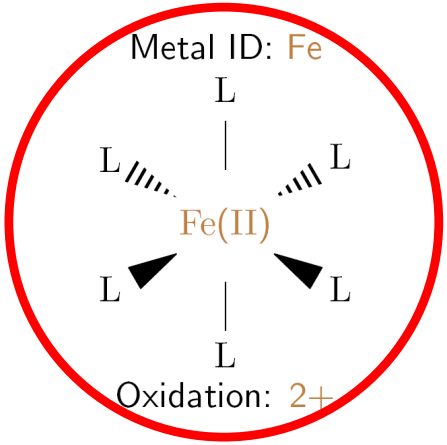

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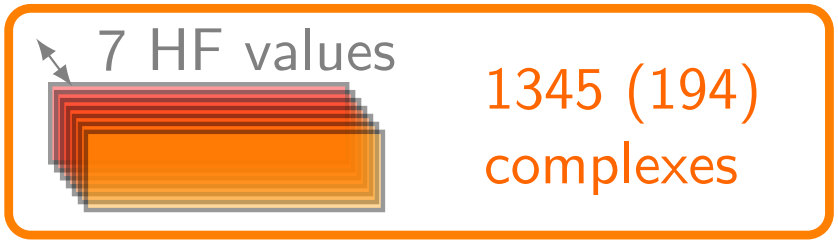

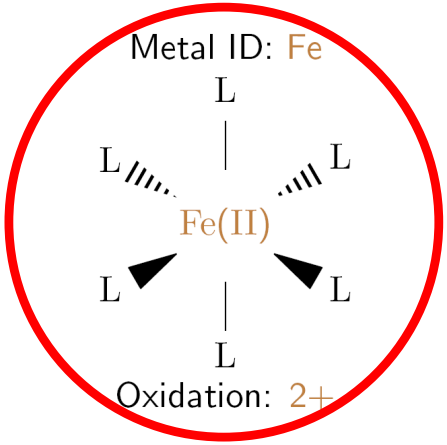

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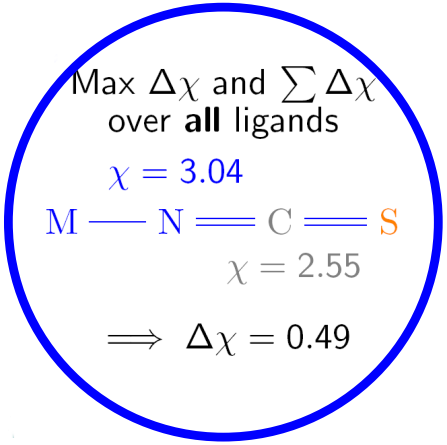

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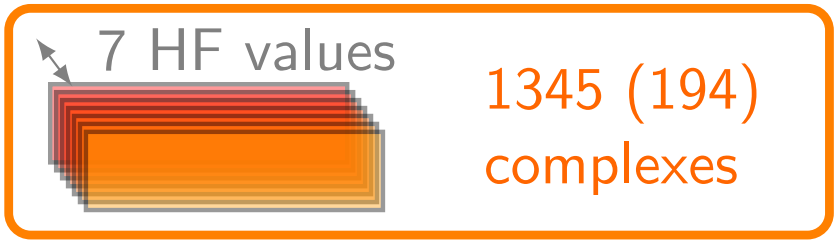

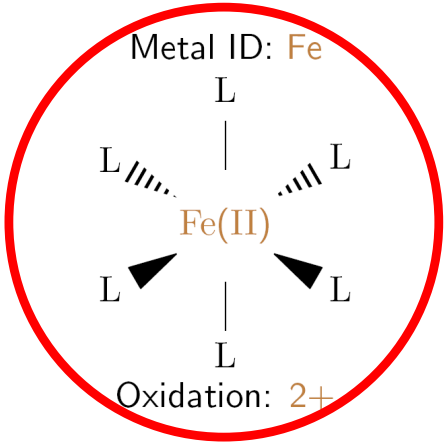

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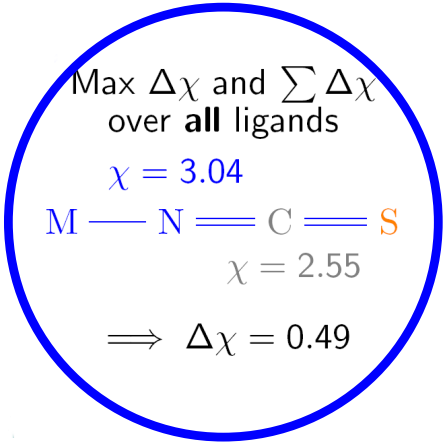

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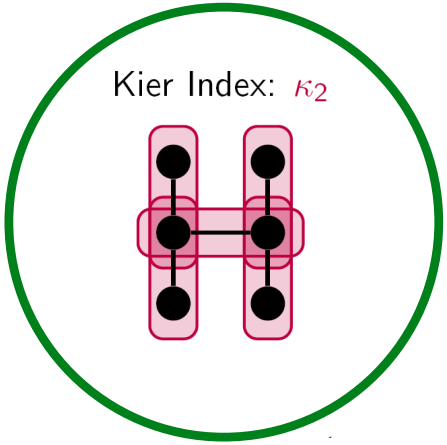

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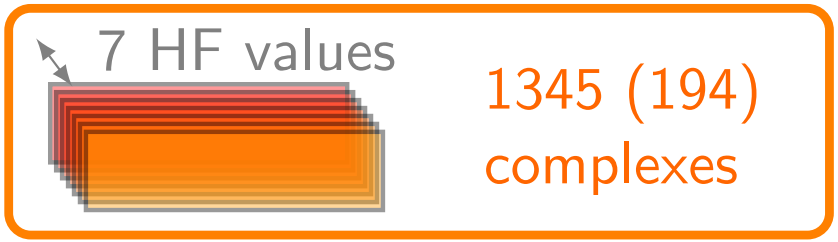

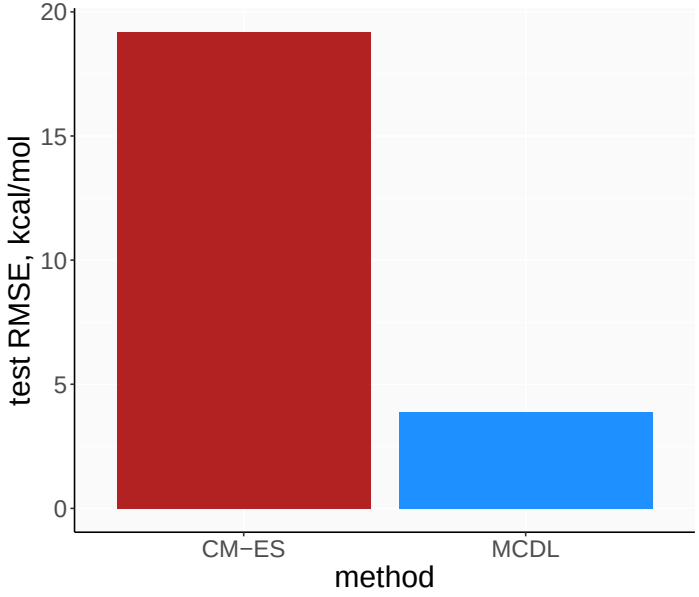

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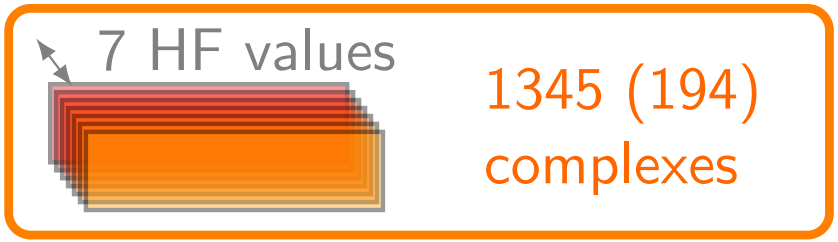

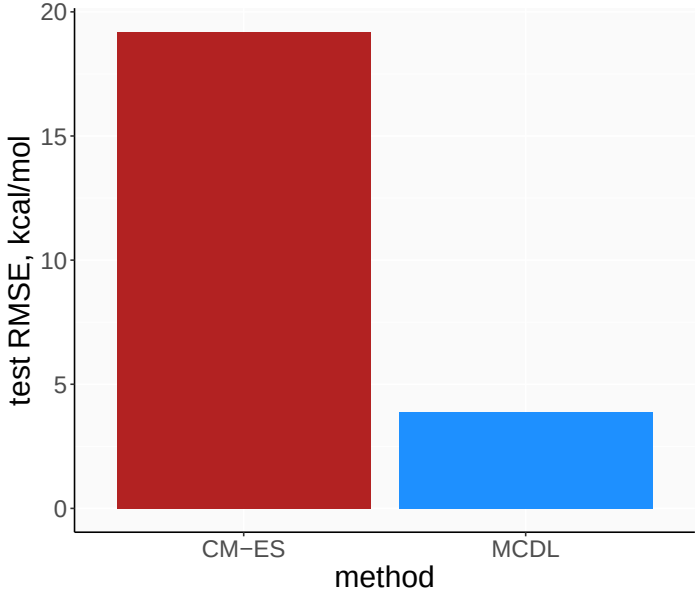

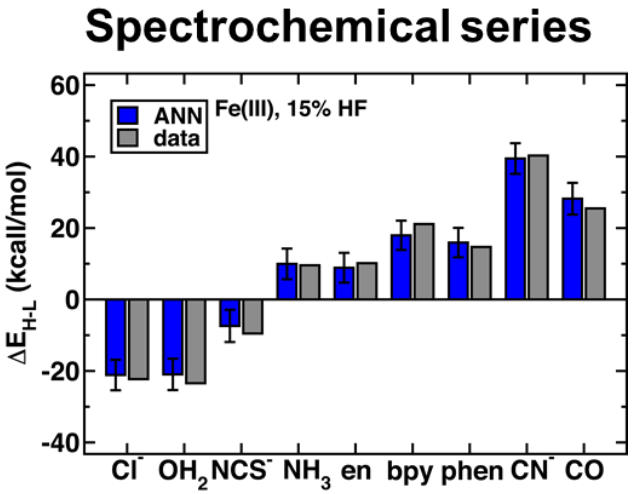

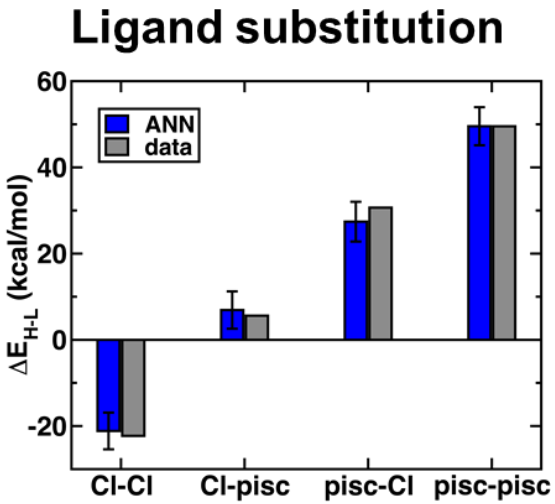

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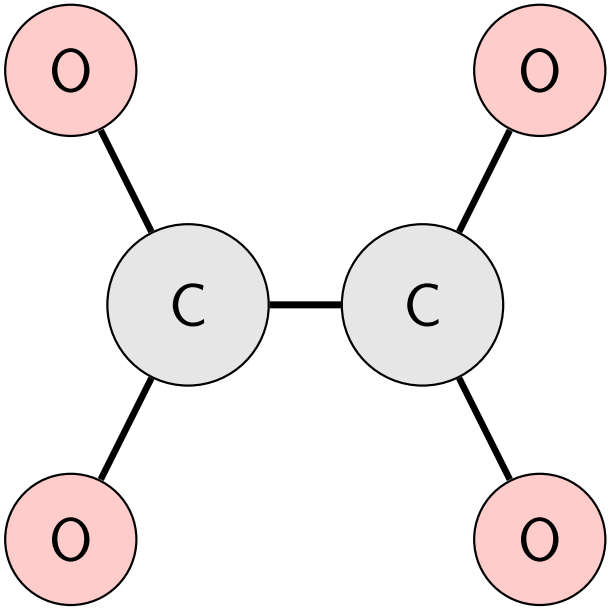

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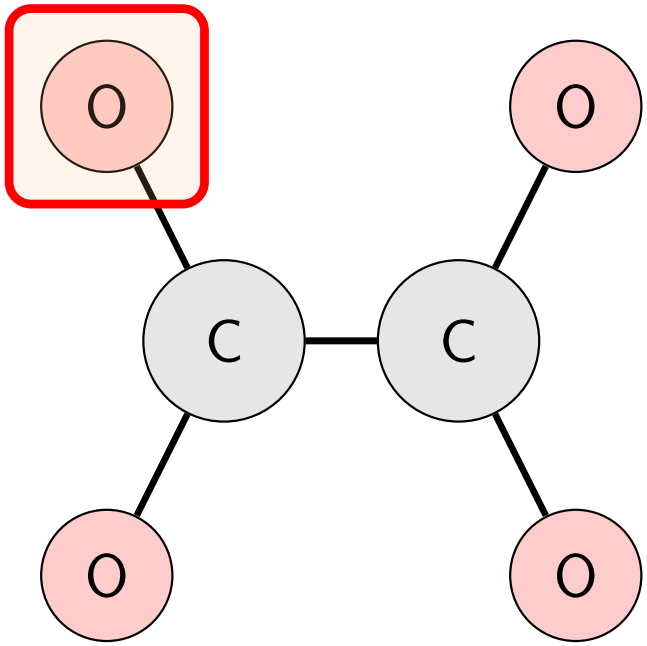

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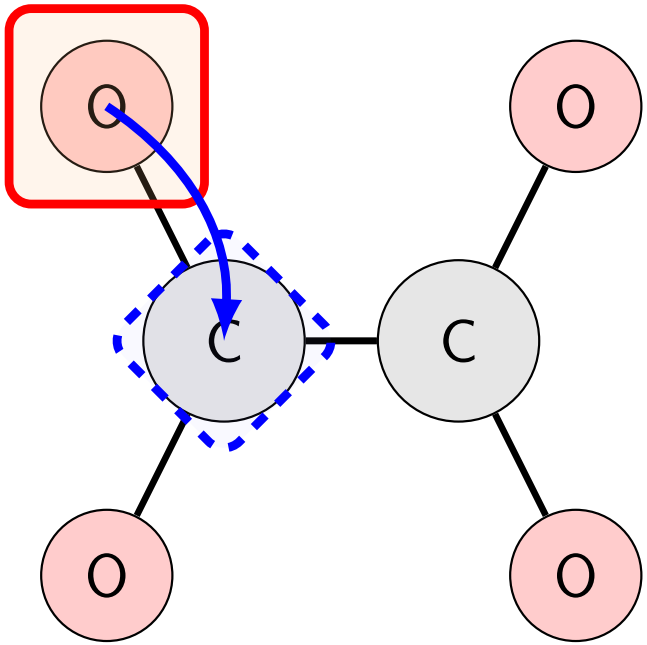

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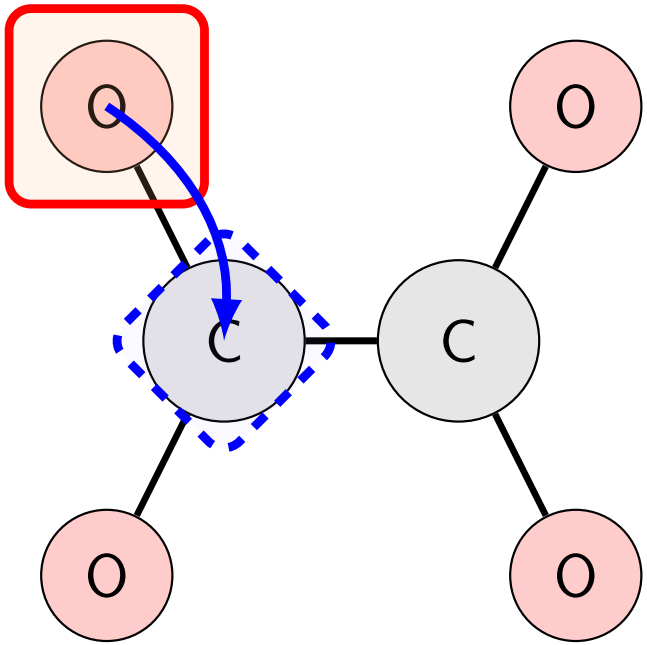

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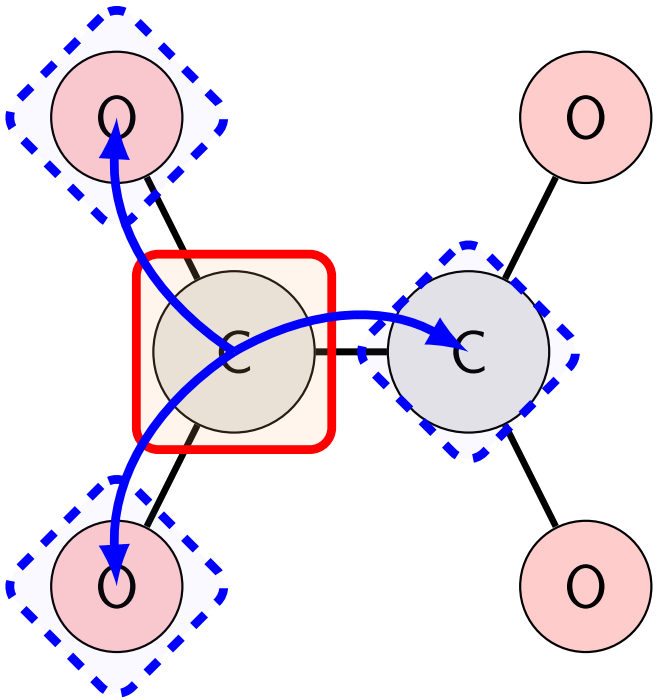

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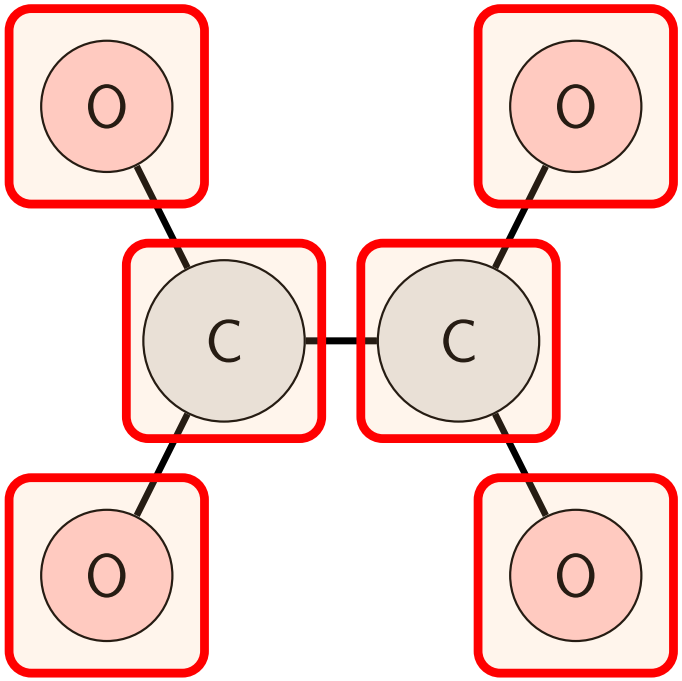

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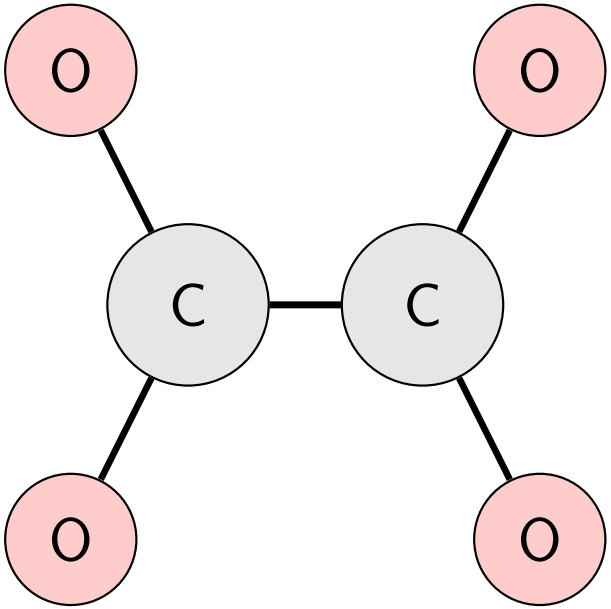

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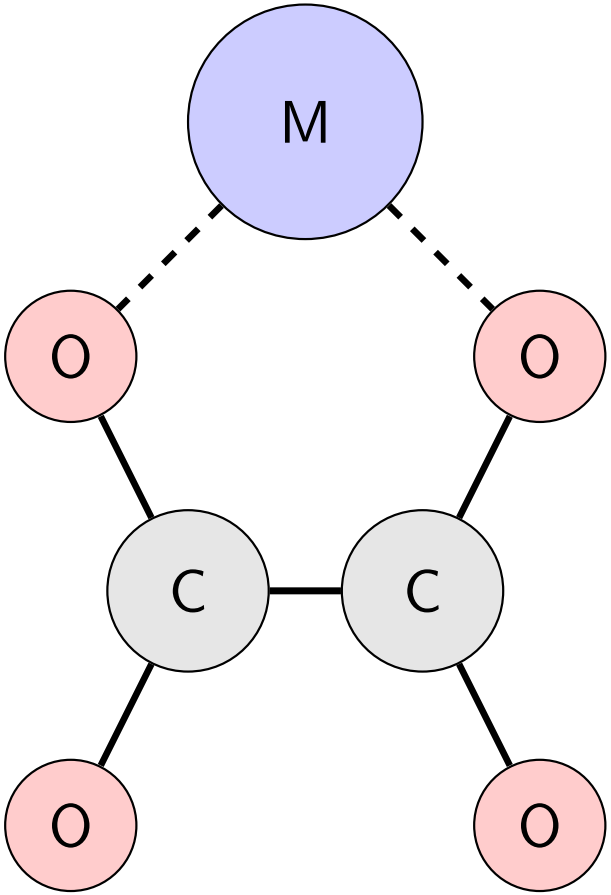

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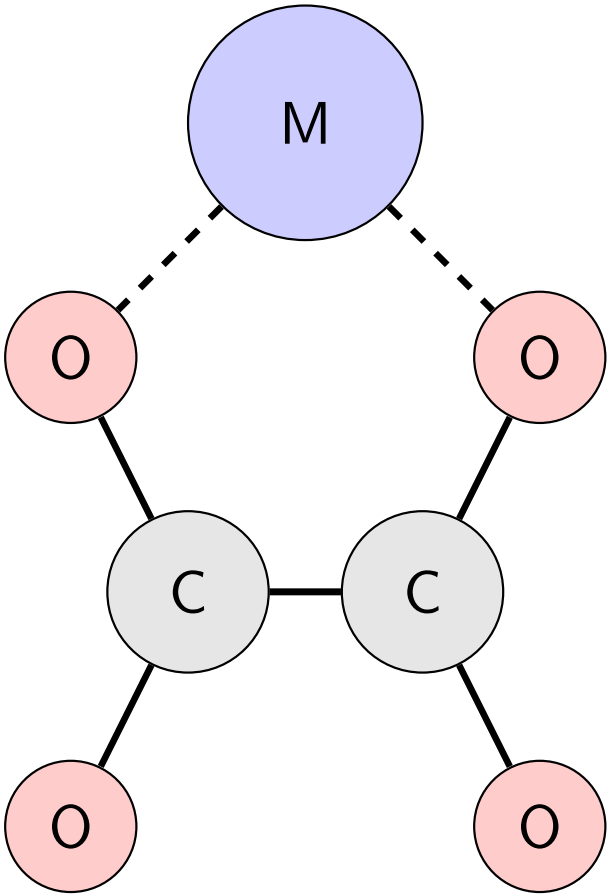

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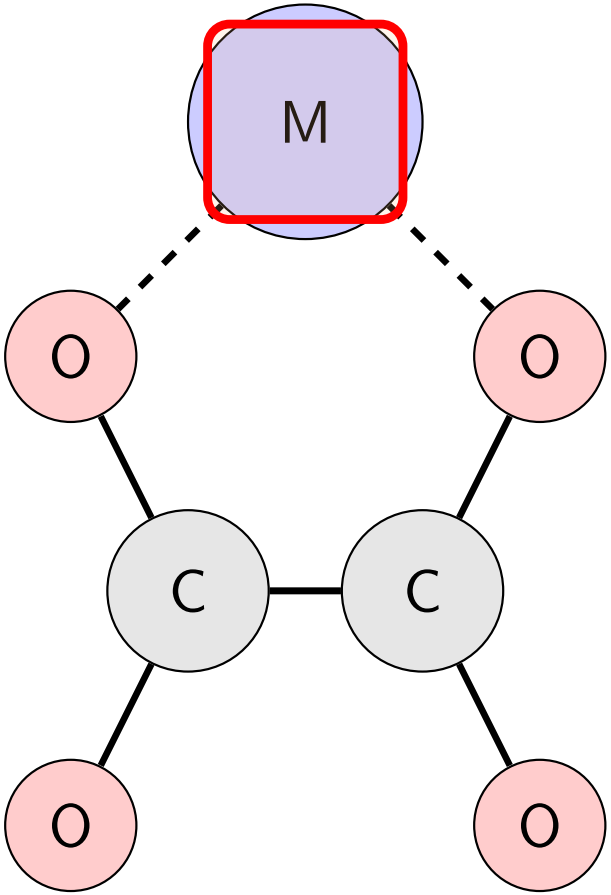

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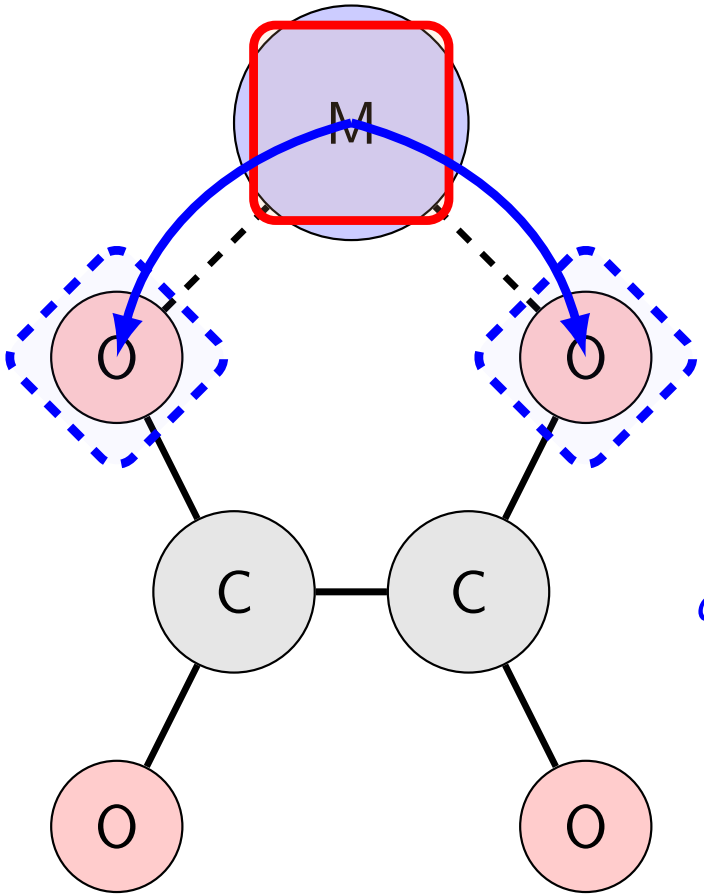

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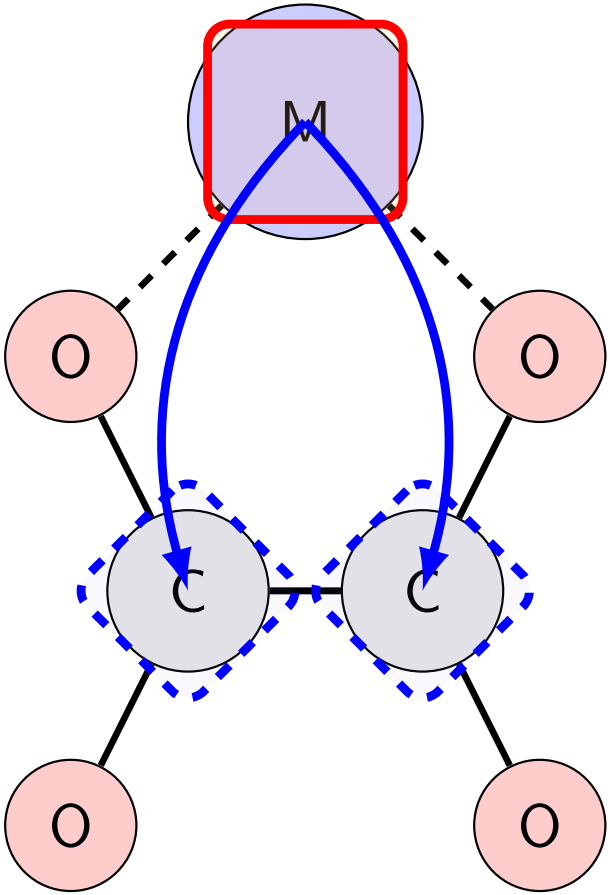
$$d_1 : \sum_{M,O} Z_M Z_O$$

[2] Janet, J.P., and Kulik, H.J., *arXiv*, 1708.06017, 2017.

RAC descriptors

RACs based on autocorrelations[2]



How to adapt to TM complexes?

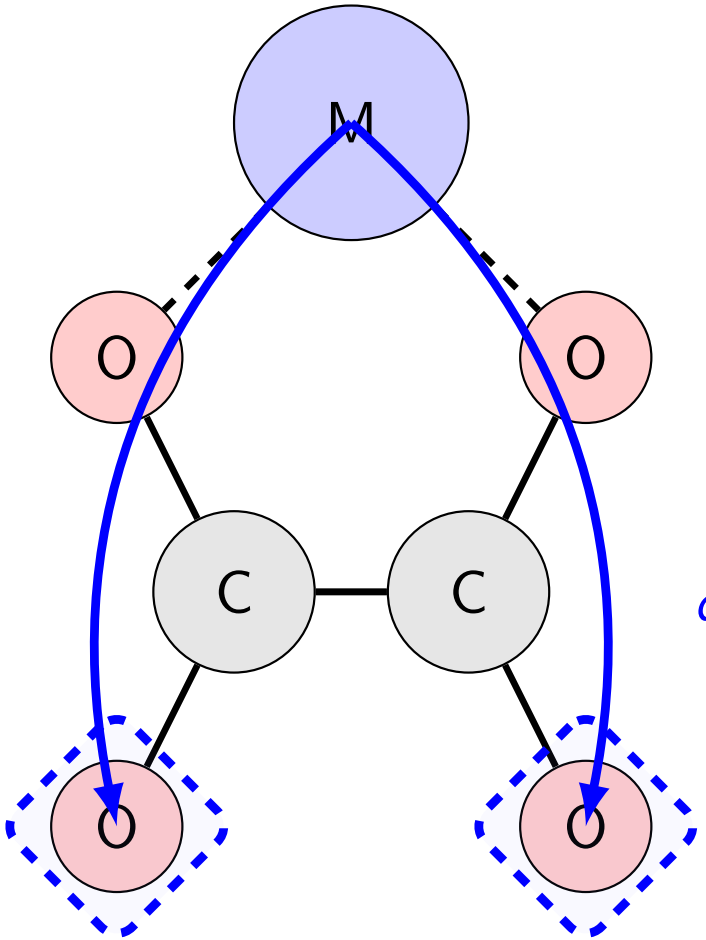
restrict the scope to focus on *near-metal atoms*

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

[2] Janet, J.P., and Kulik, H.J., *arXiv*, 1708.06017, 2017.

RAC descriptors

RACs based on autocorrelations[2]



How to adapt to TM complexes?

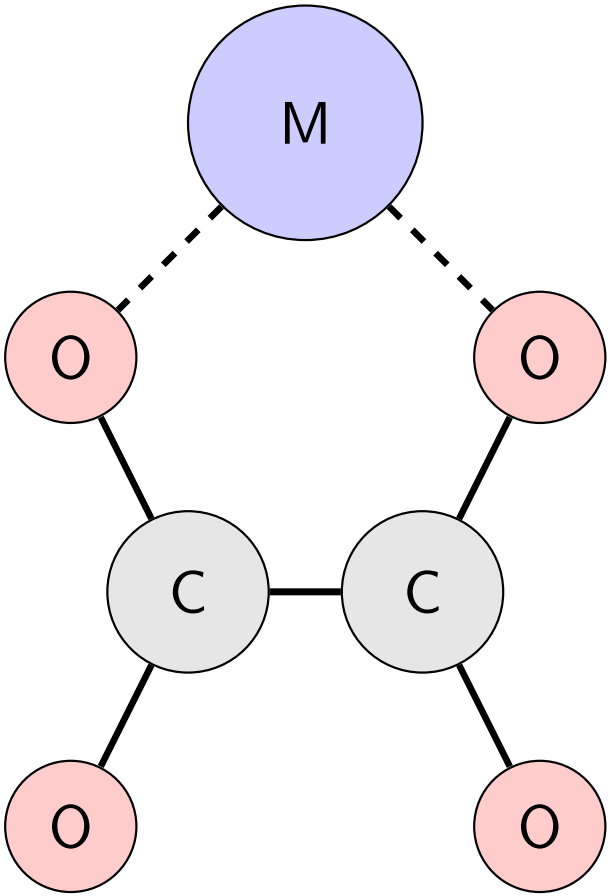
restrict the scope to focus on *near-metal atoms*

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

[2] Janet, J.P., and Kulik, H.J., *arXiv*, 1708.06017, 2017.

RAC descriptors

RACs based on autocorrelations[2]



How to adapt to TM complexes?

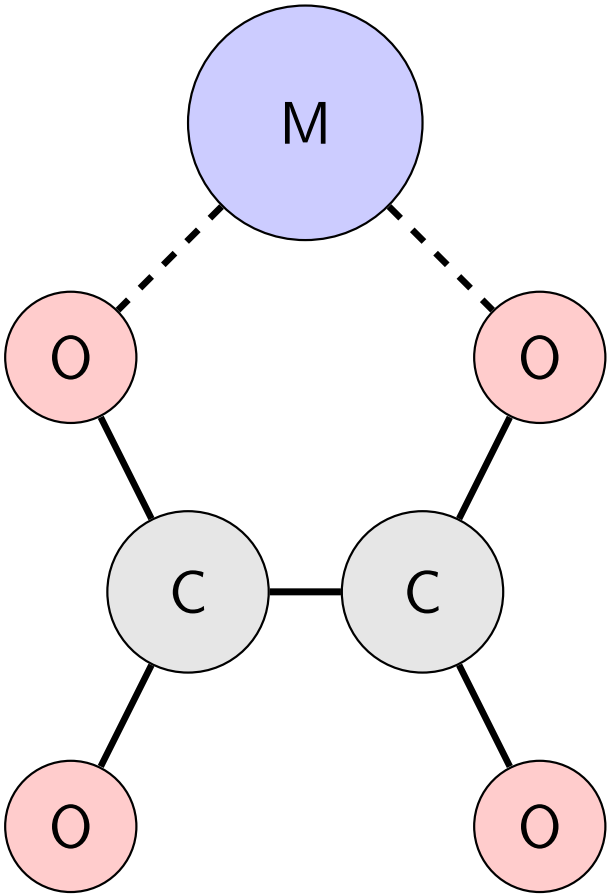
restrict the scope to focus on *near-metal atoms*

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

[2] Janet, J.P., and Kulik, H.J., *arXiv*, 1708.06017, 2017.

RAC descriptors

RACs based on autocorrelations[2]



How to adapt to TM complexes?

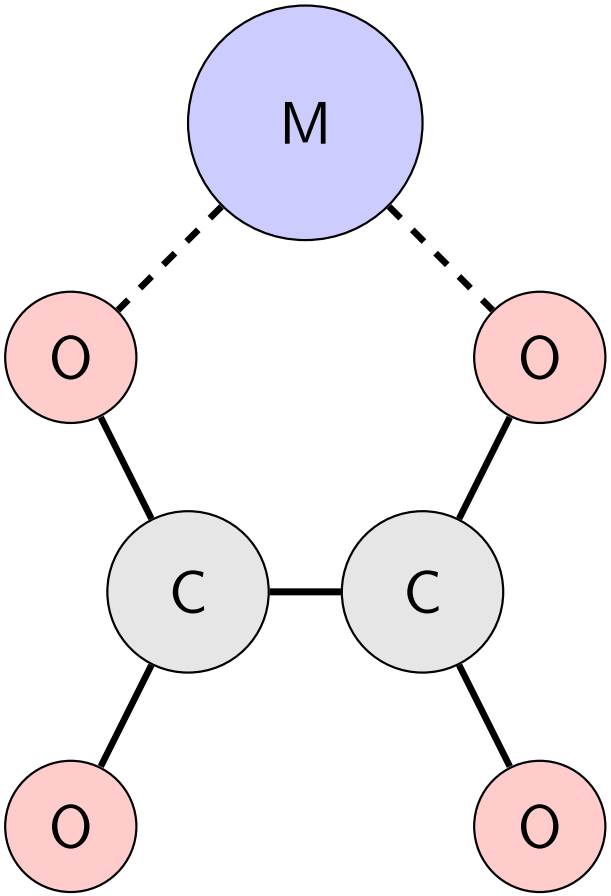
restrict the scope to focus on *near-metal atoms*

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

[2] Janet, J.P., and Kulik, H.J., *arXiv*, 1708.06017, 2017.

RAC descriptors

RACs based on autocorrelations[2]



How to adapt to TM complexes?

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

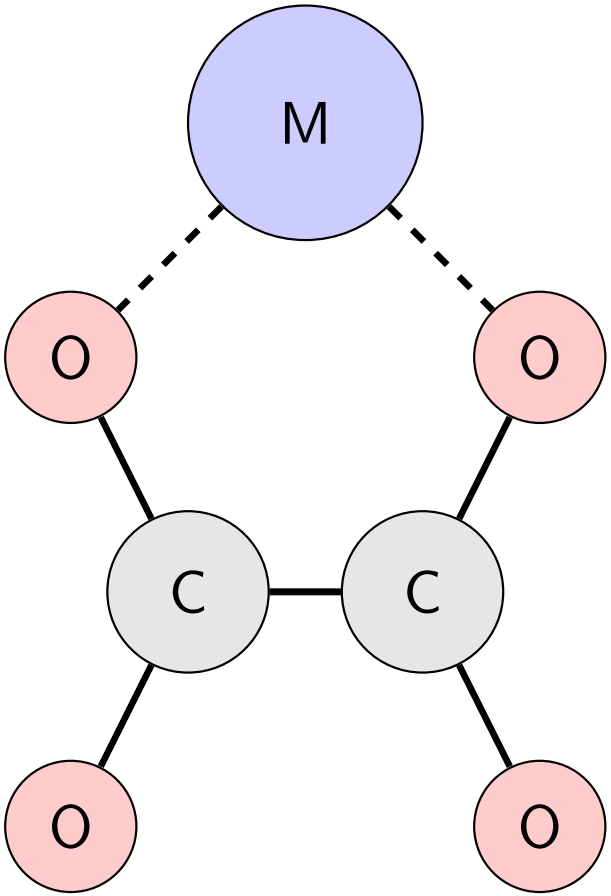
$$d_3 : \sum_{M,O} Z_M Z_O (Z_i - Z_j)$$

properties: T, χ, Z, I, S

[2] Janet, J.P., and Kulik, H.J., *arXiv*, 1708.06017, 2017.

RAC descriptors

RACs based on autocorrelations[2]



How to adapt to TM complexes?

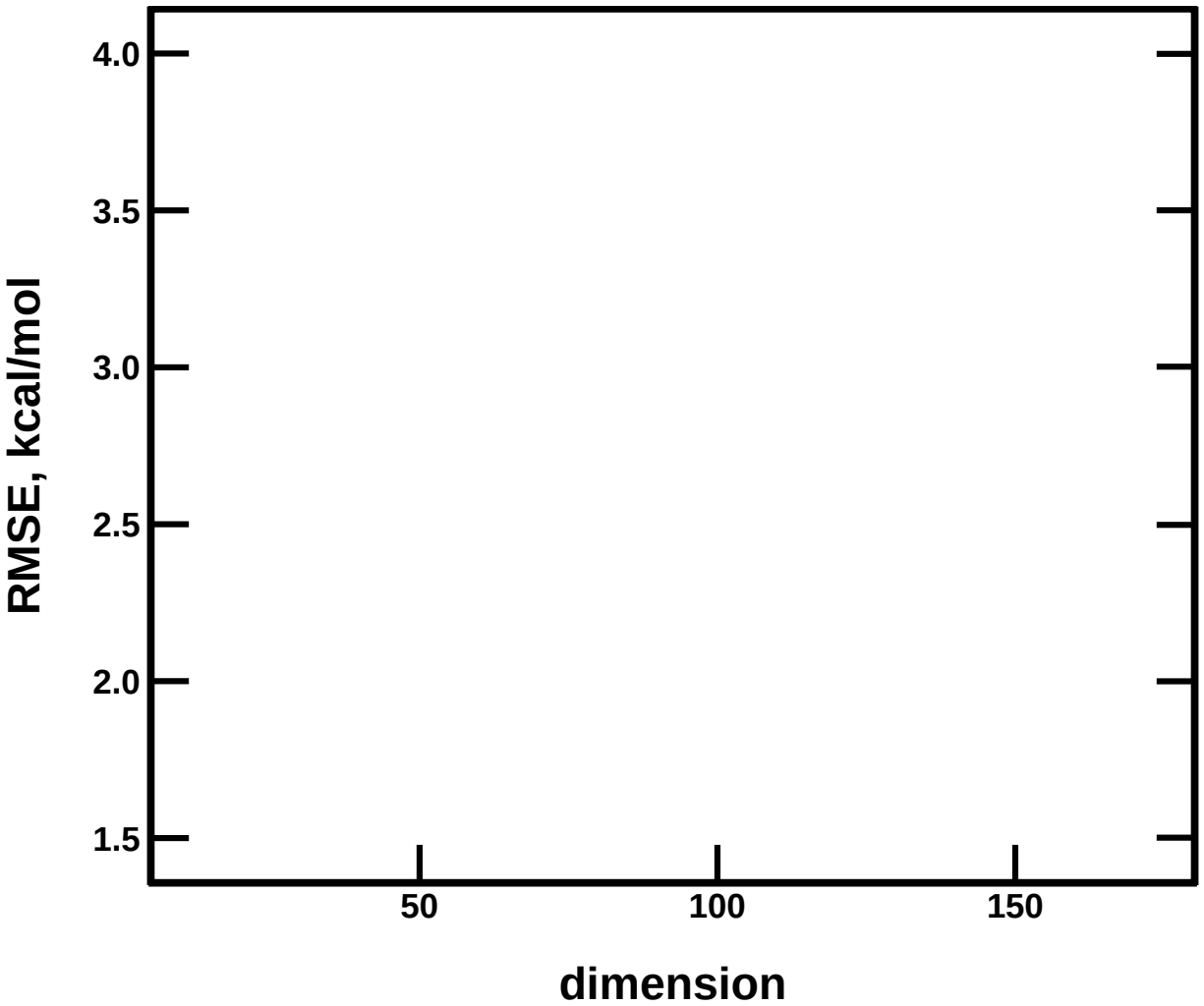
restrict the scope to focus on *near-metal atoms*

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

$\boxed{\sim 160 \text{ features in total}}$

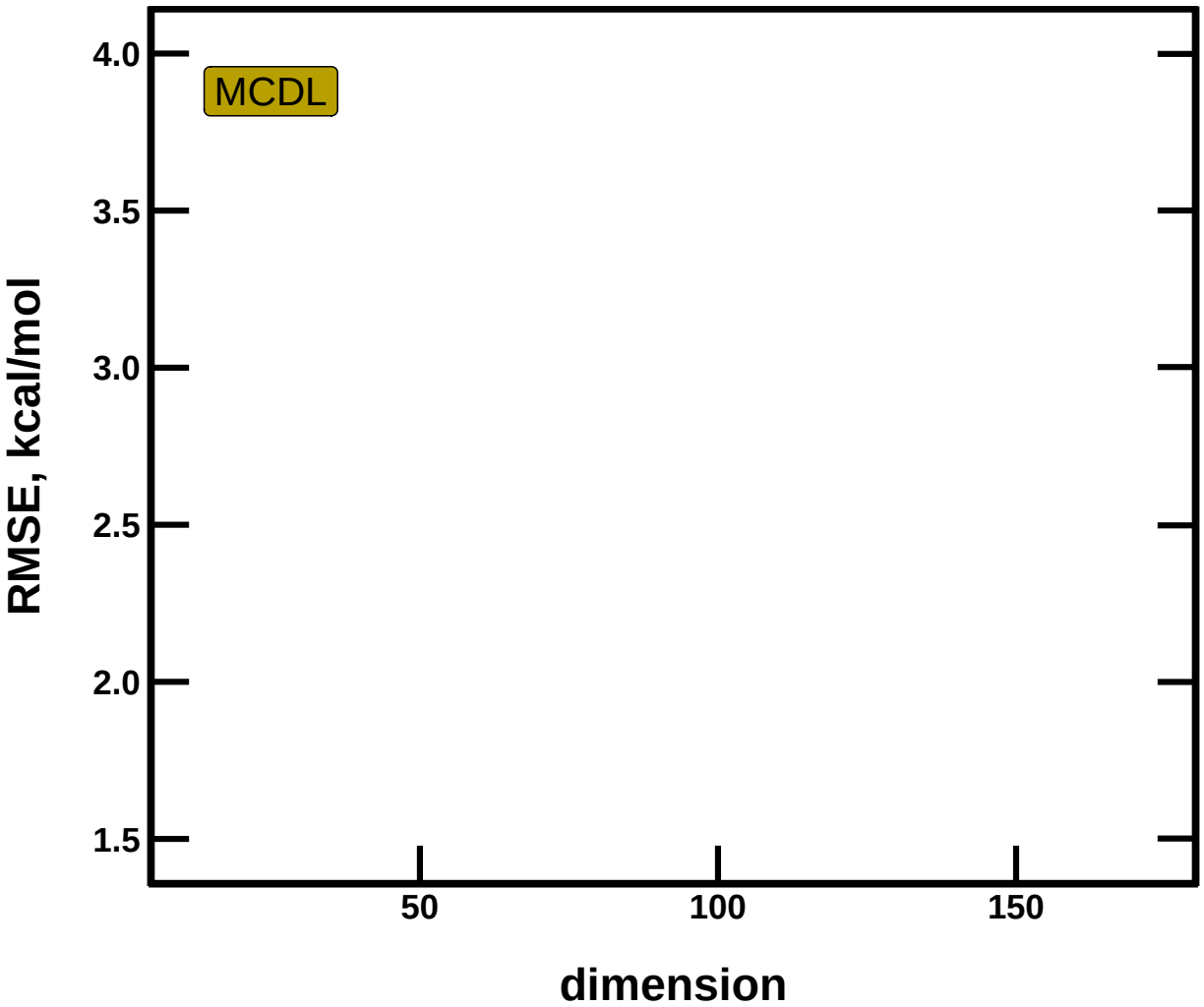
[2] Janet, J.P., and Kulik, H.J., *arXiv*, 1708.06017, 2017.

Feature selection



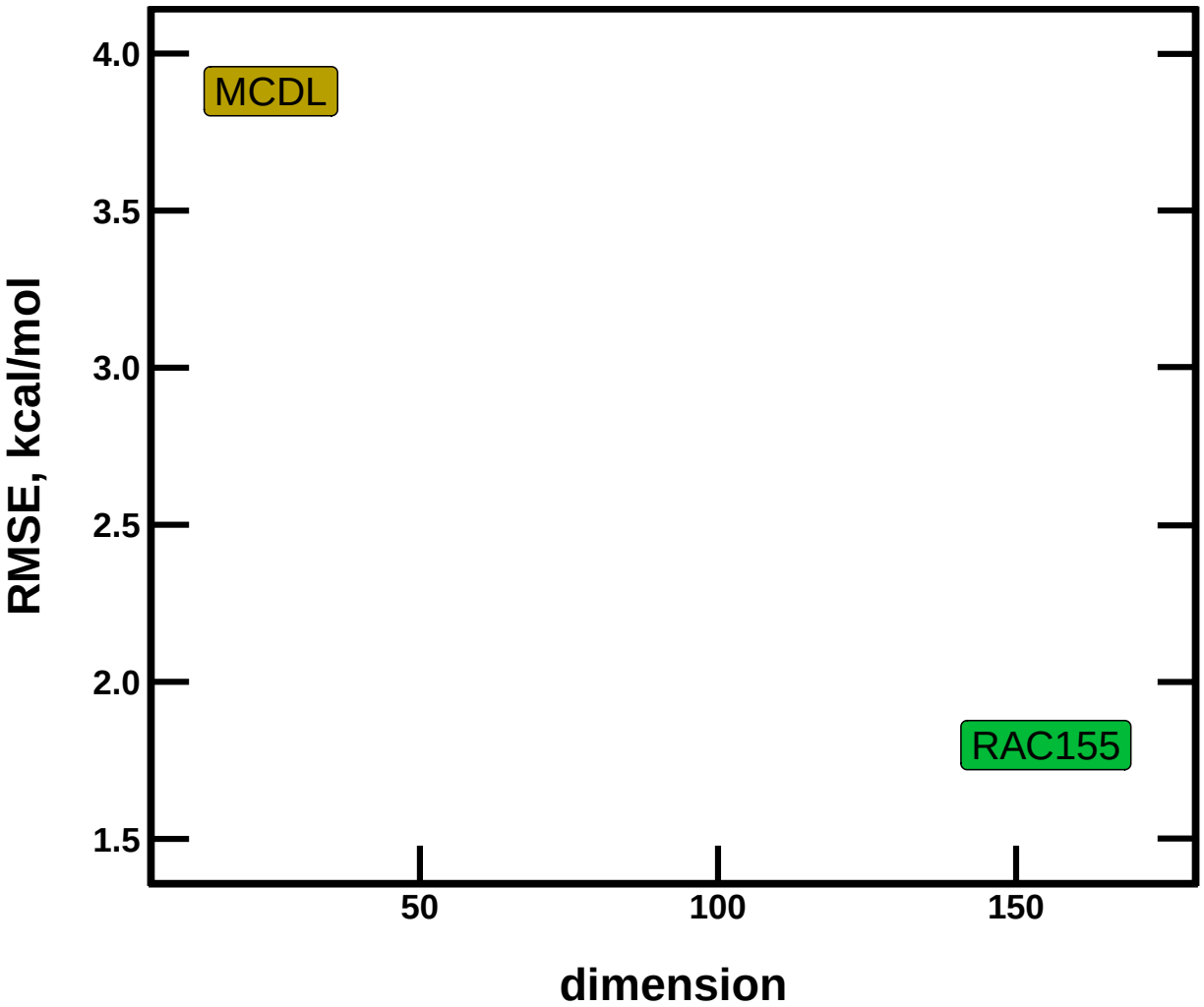
Janet, J.P., and Kulik, H.J., *arXiv*, 1708.06017, 2017.

Feature selection



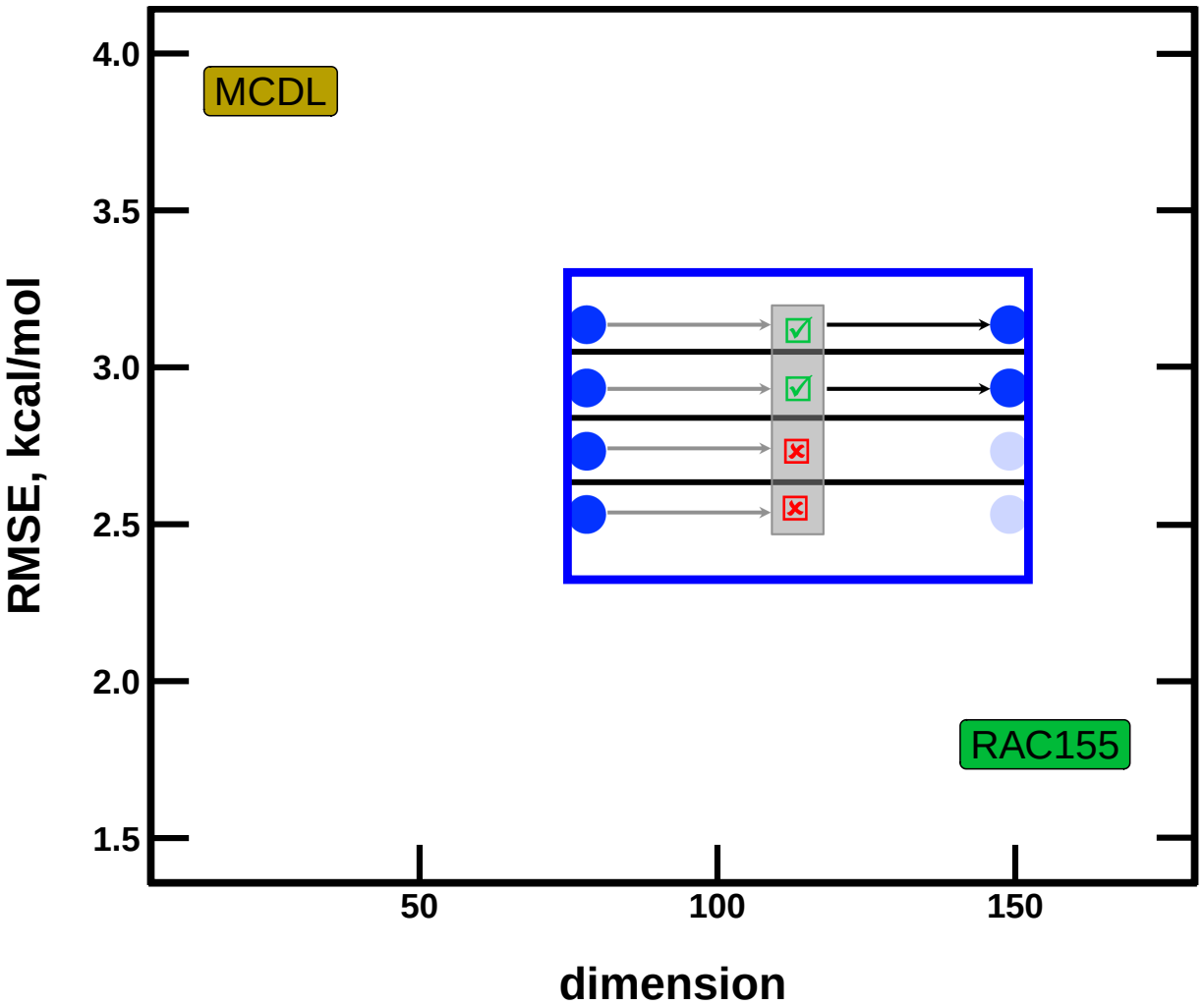
Janet, J.P., and Kulik, H.J., *arXiv*, 1708.06017, 2017.

Feature selection



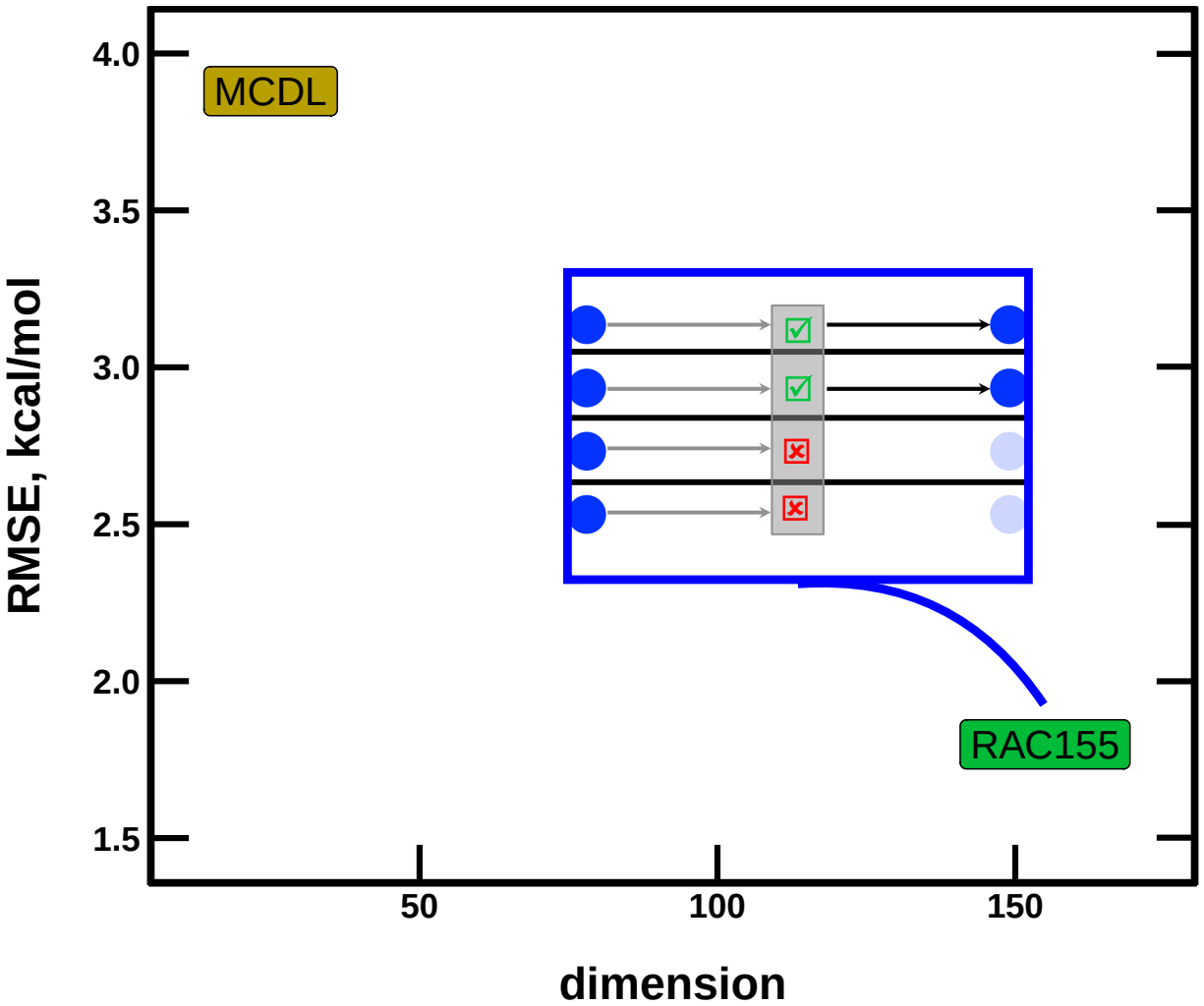
Janet, J.P., and Kulik, H.J., *arXiv*, 1708.06017, 2017.

Feature selection



Janet, J.P., and Kulik, H.J., *arXiv*, 1708.06017, 2017.

Feature selection



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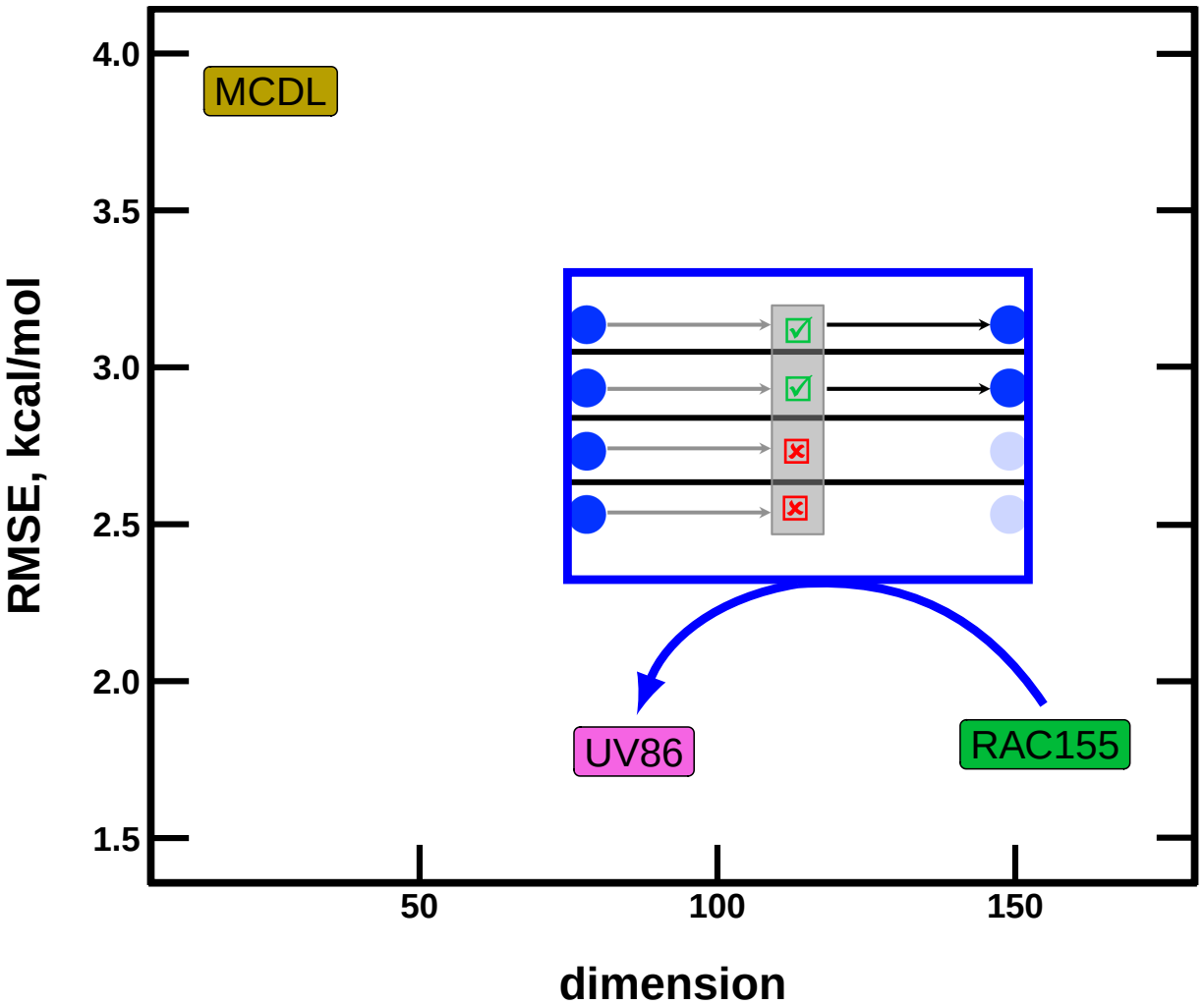
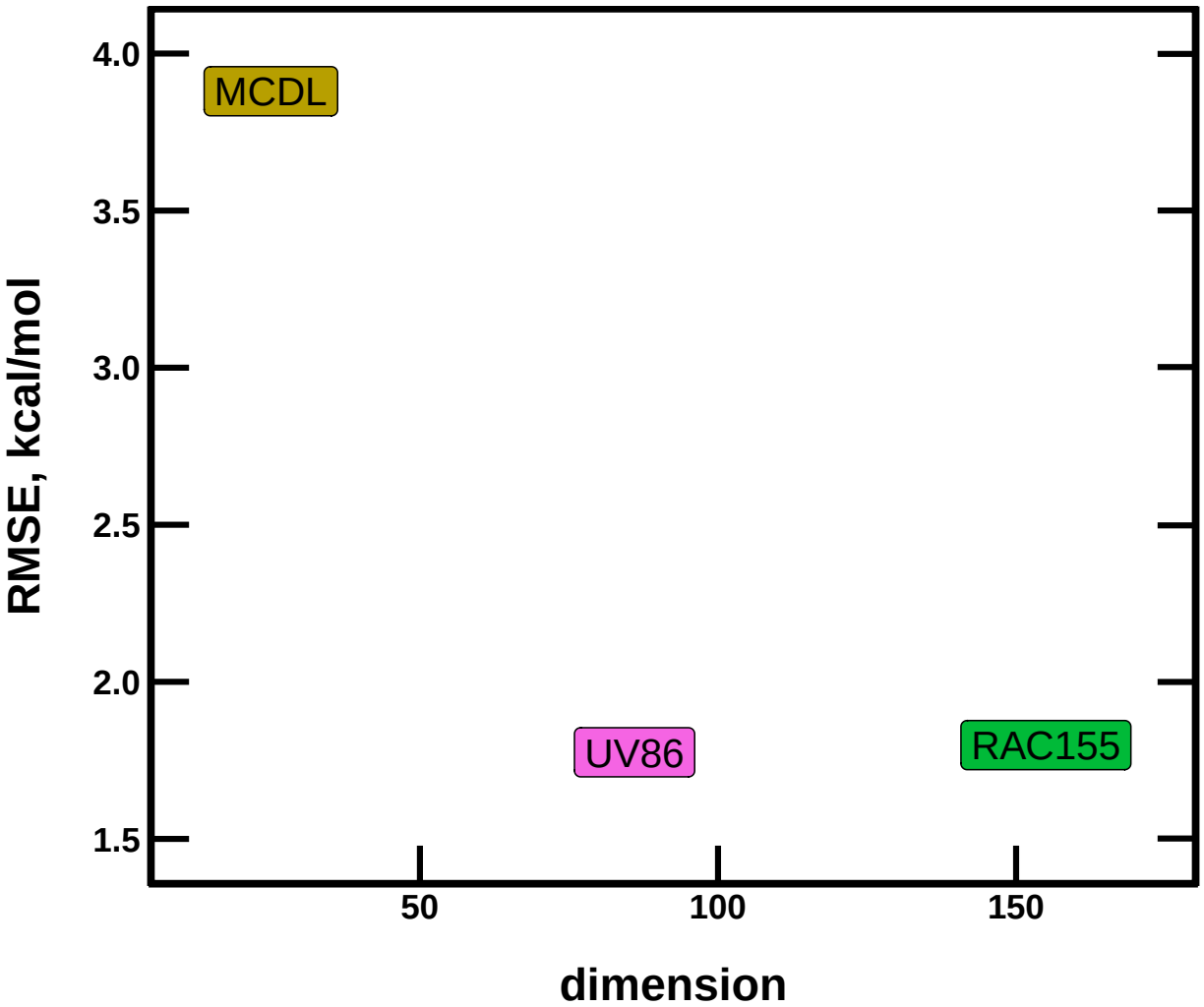
Feature selection



Janet, J.P., and Kulik, H.J., *arXiv*, 1708.06017, 2017.

Feature selection



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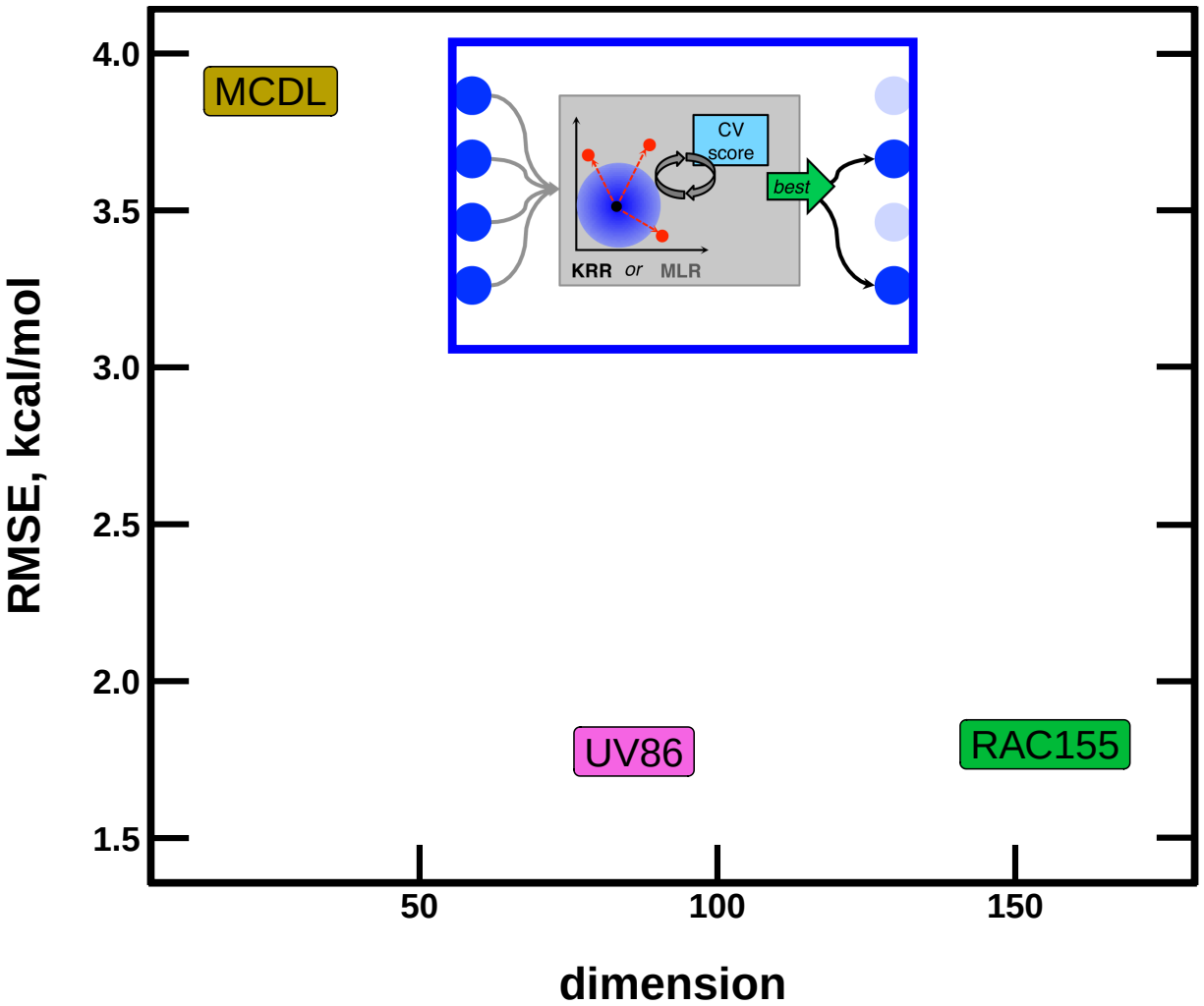

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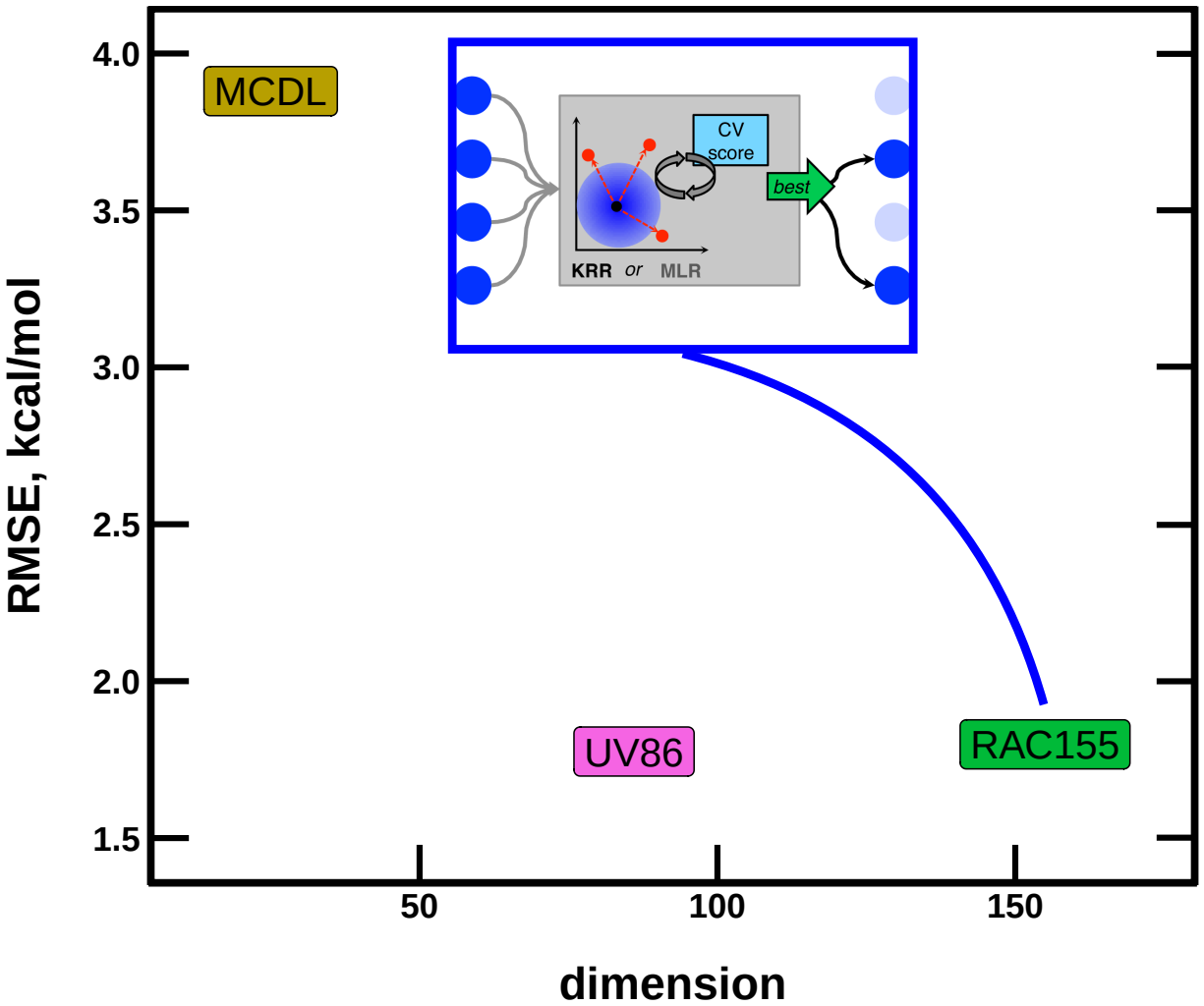

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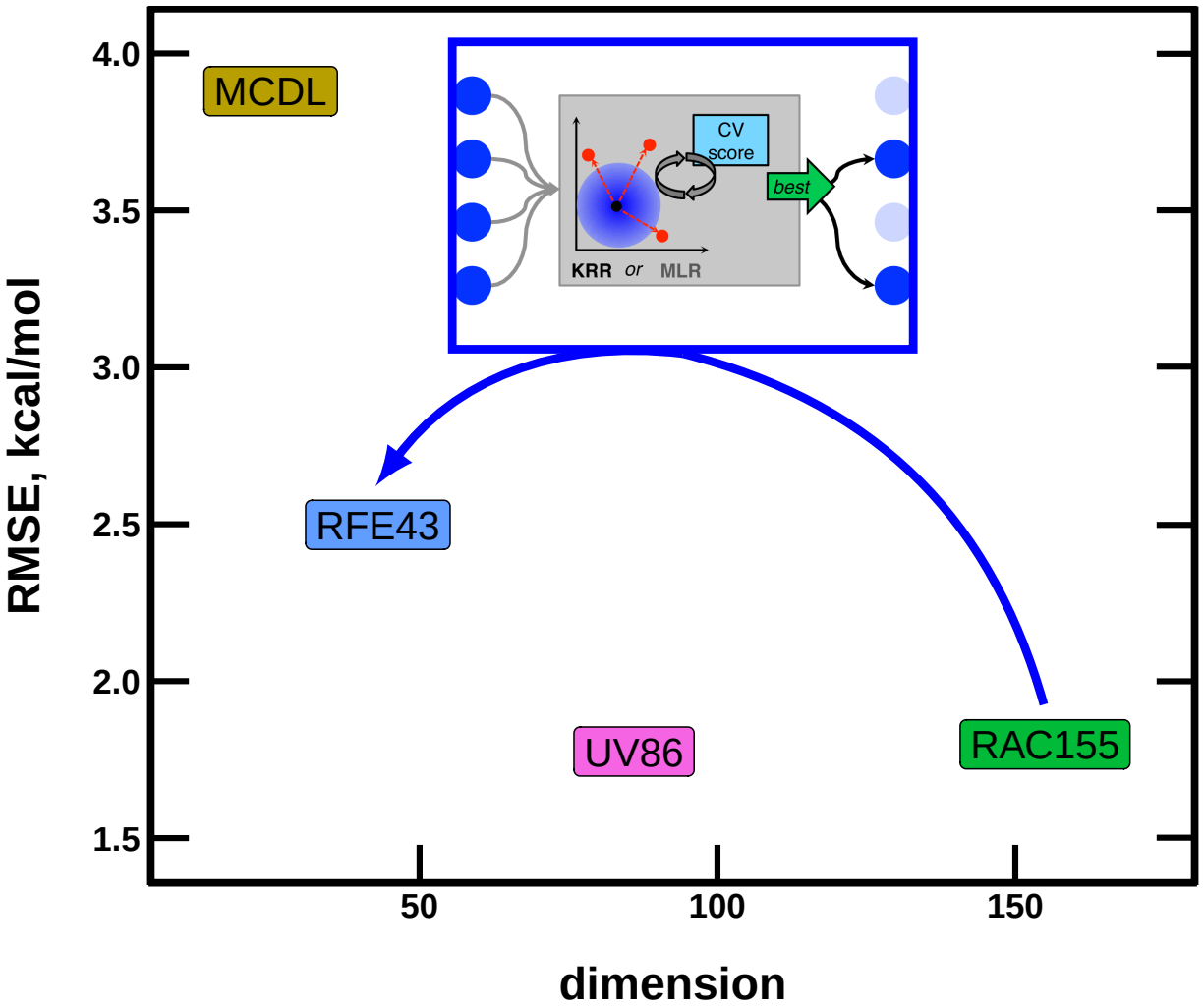

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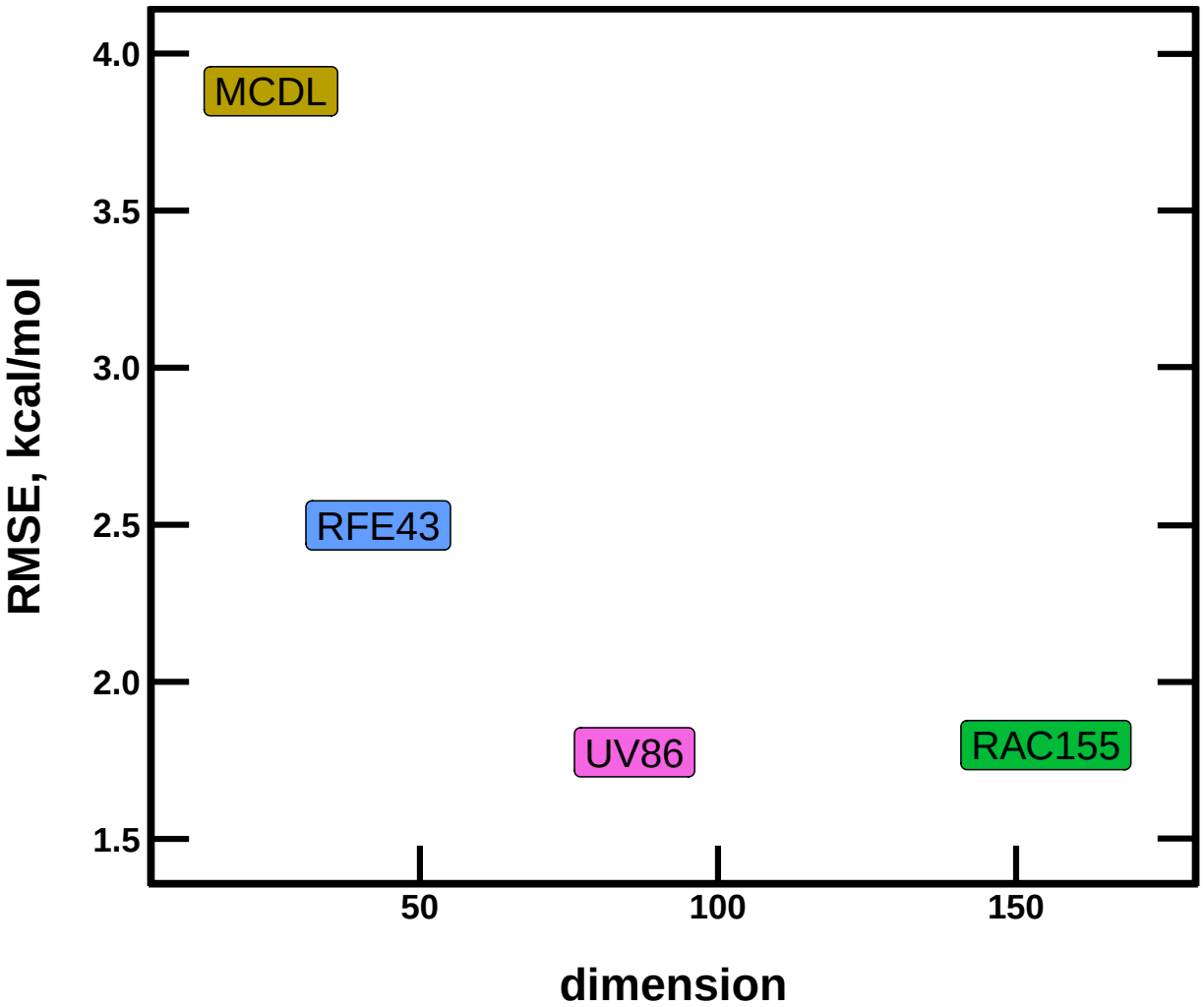

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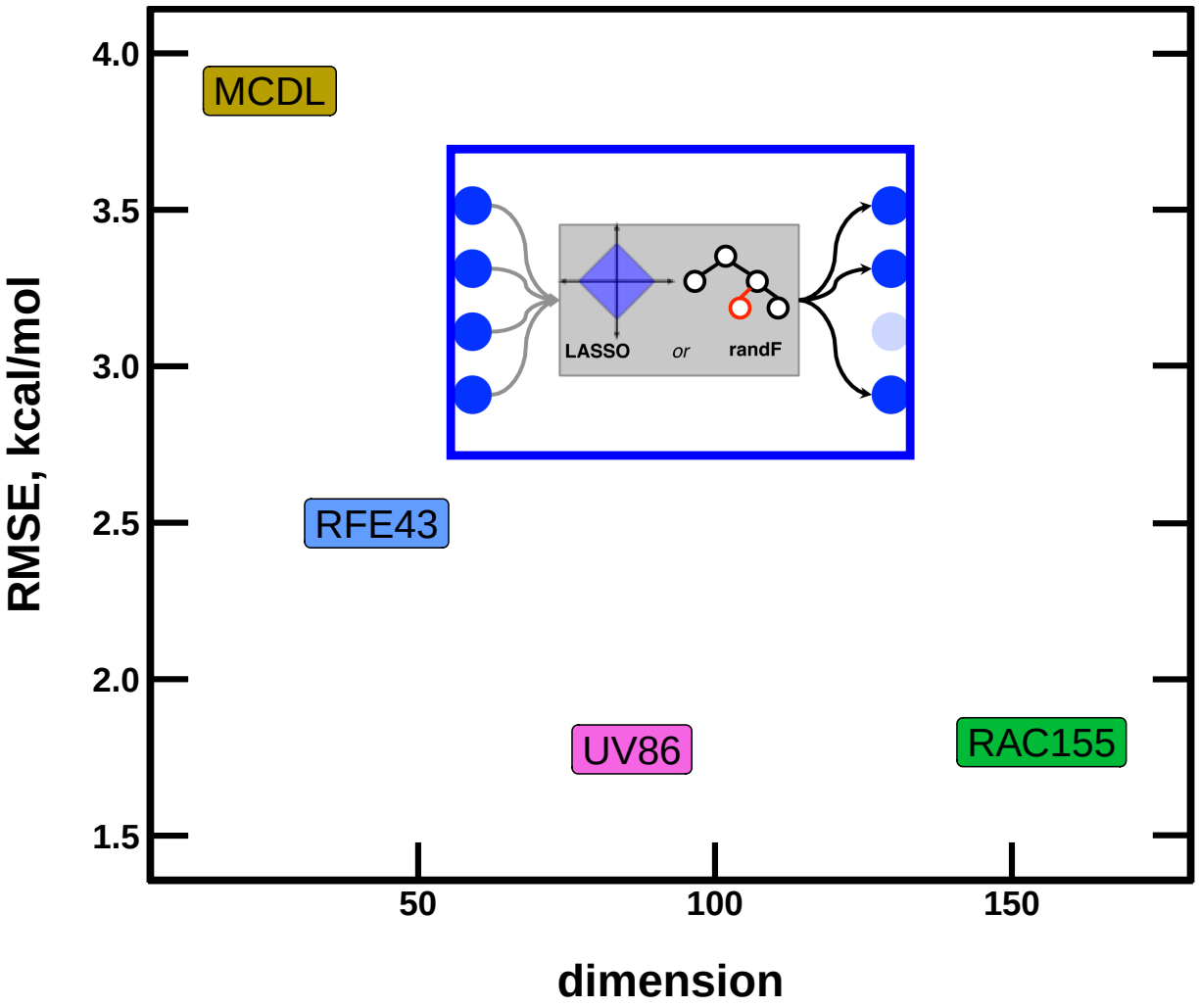
Feature selection



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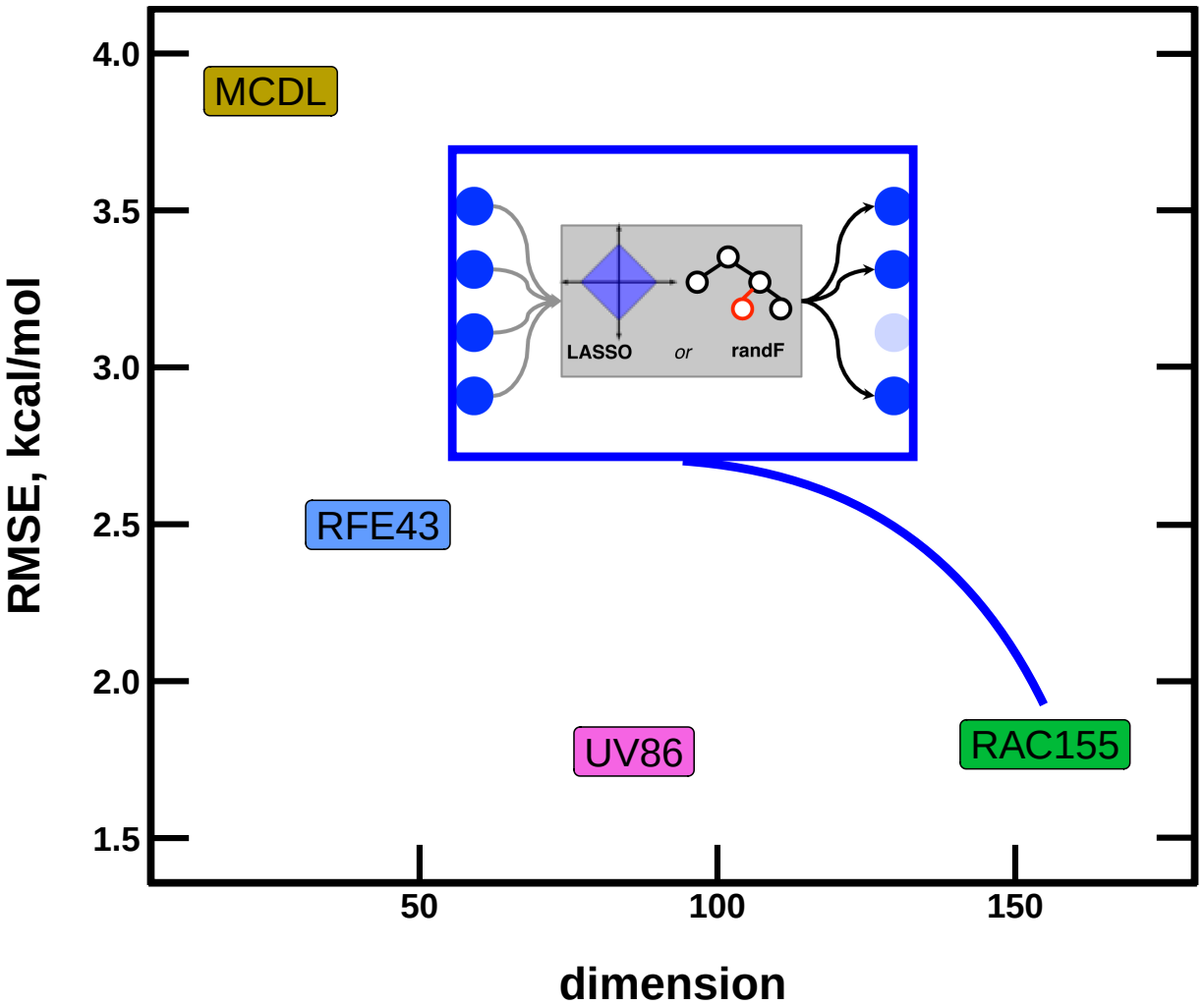
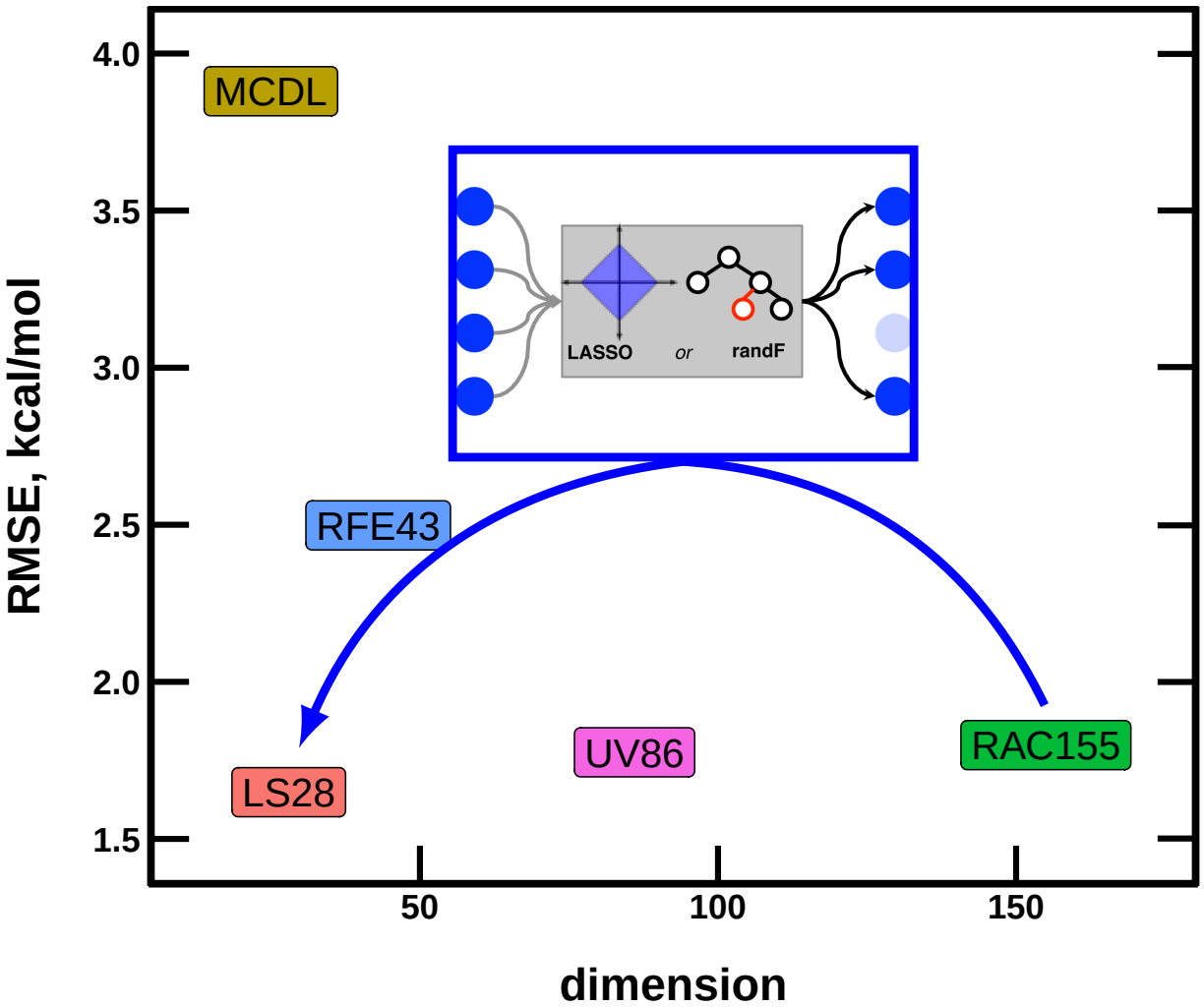
Feature selection



Janet, J.P., and Kulik, H.J., *arXiv*, 1708.06017, 2017.

Feature selection



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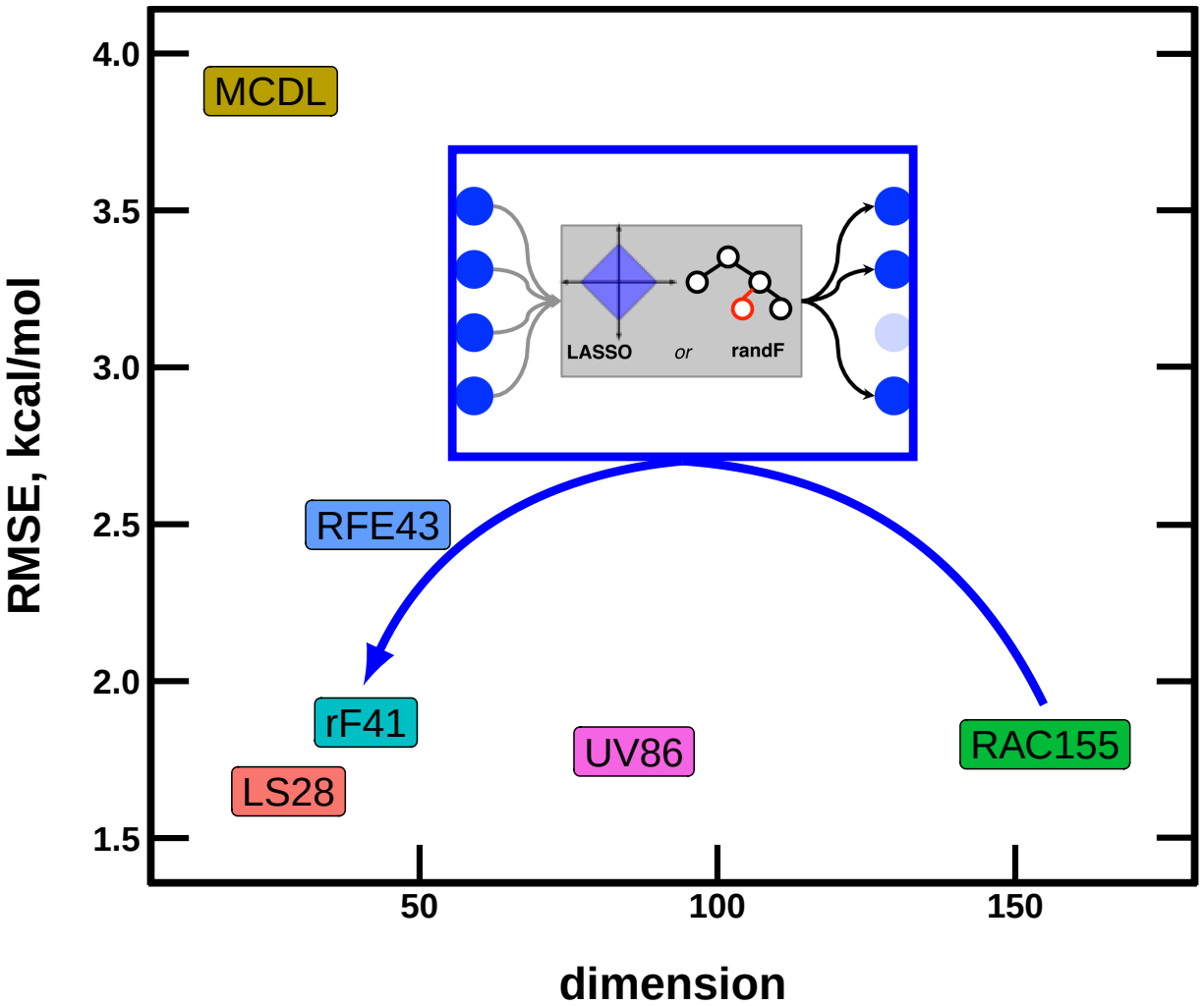
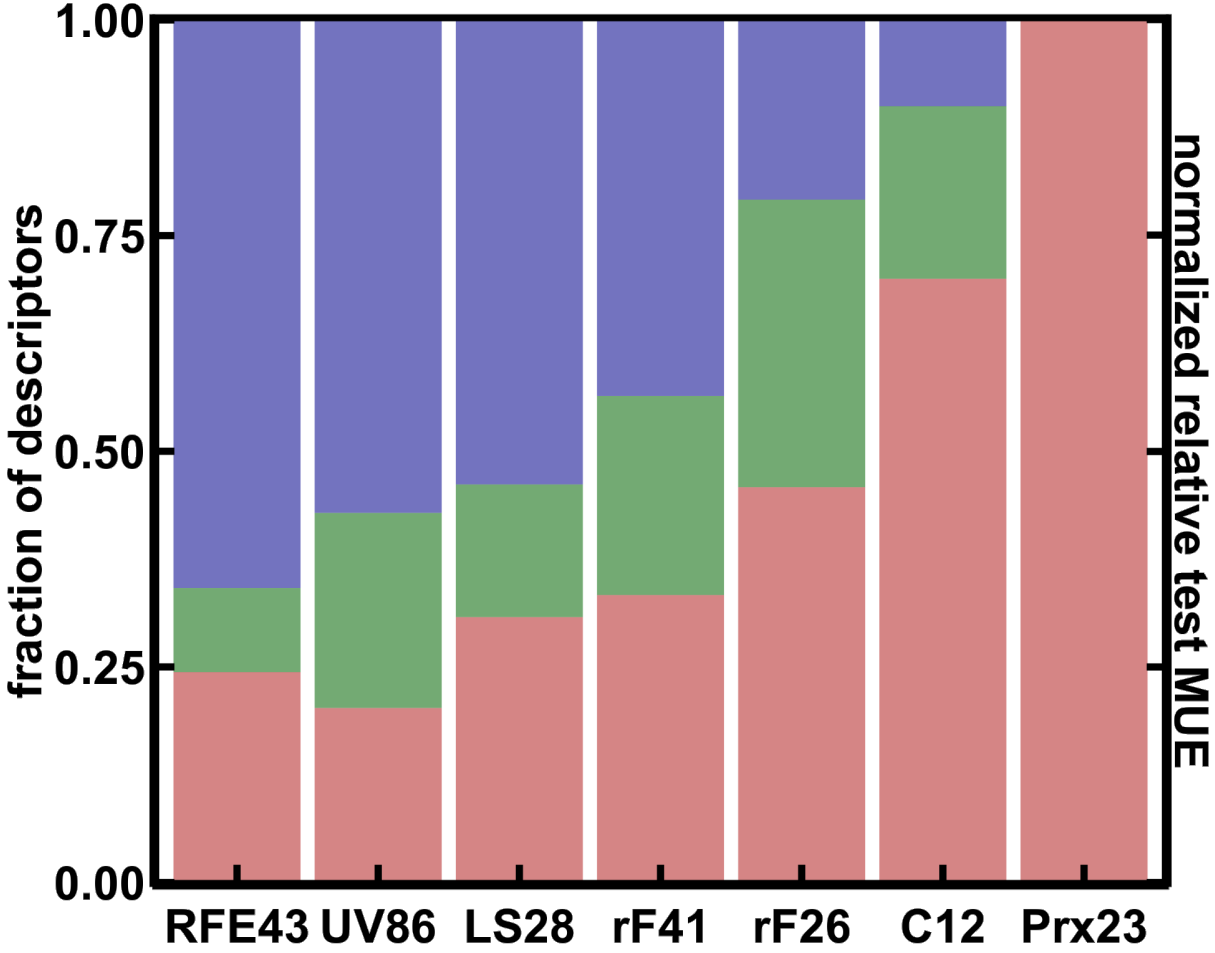
Feature selection



Janet, J.P., and Kulik, H.J., *arXiv*, 1708.06017, 2017.

How local is too local?



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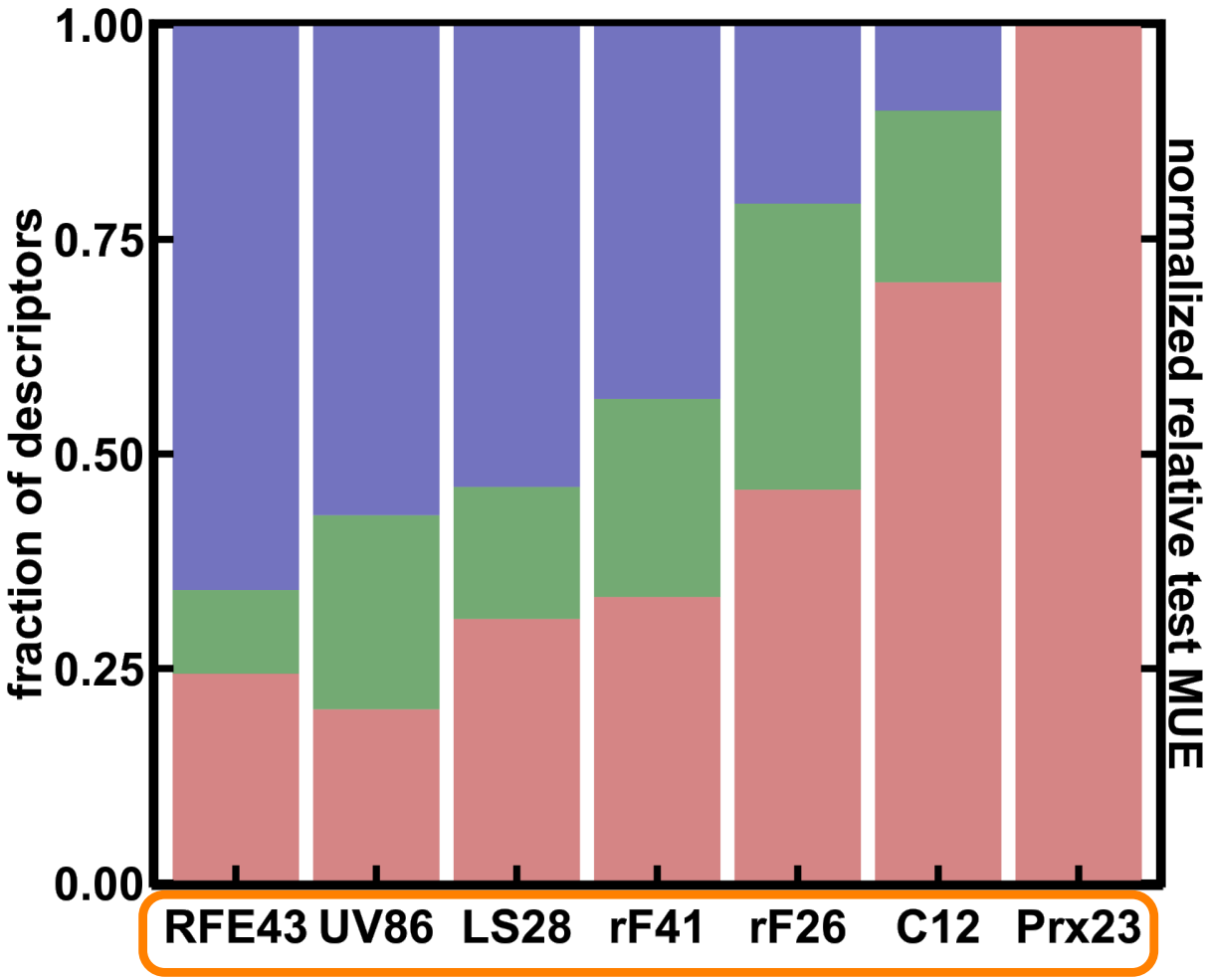

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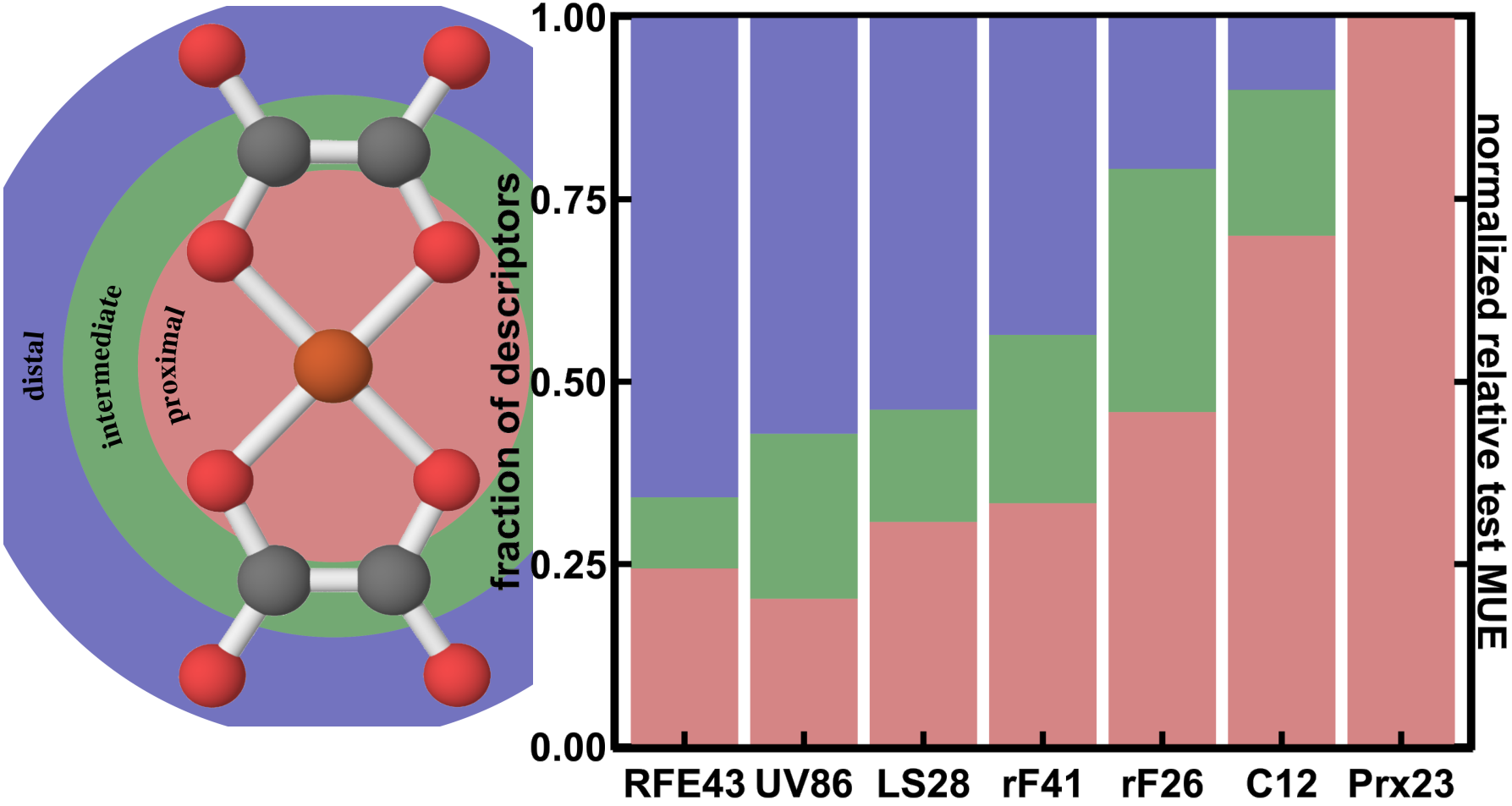

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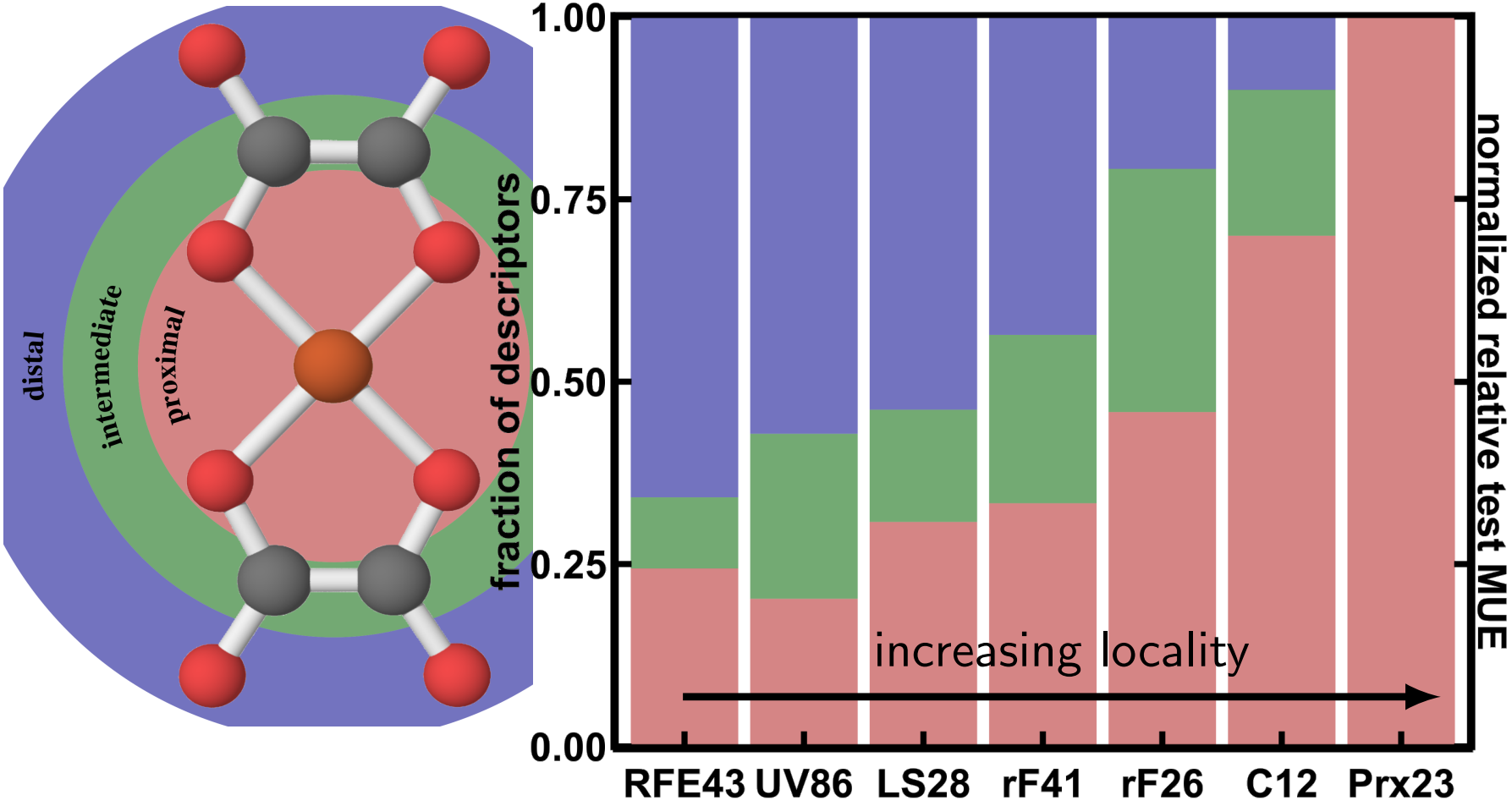

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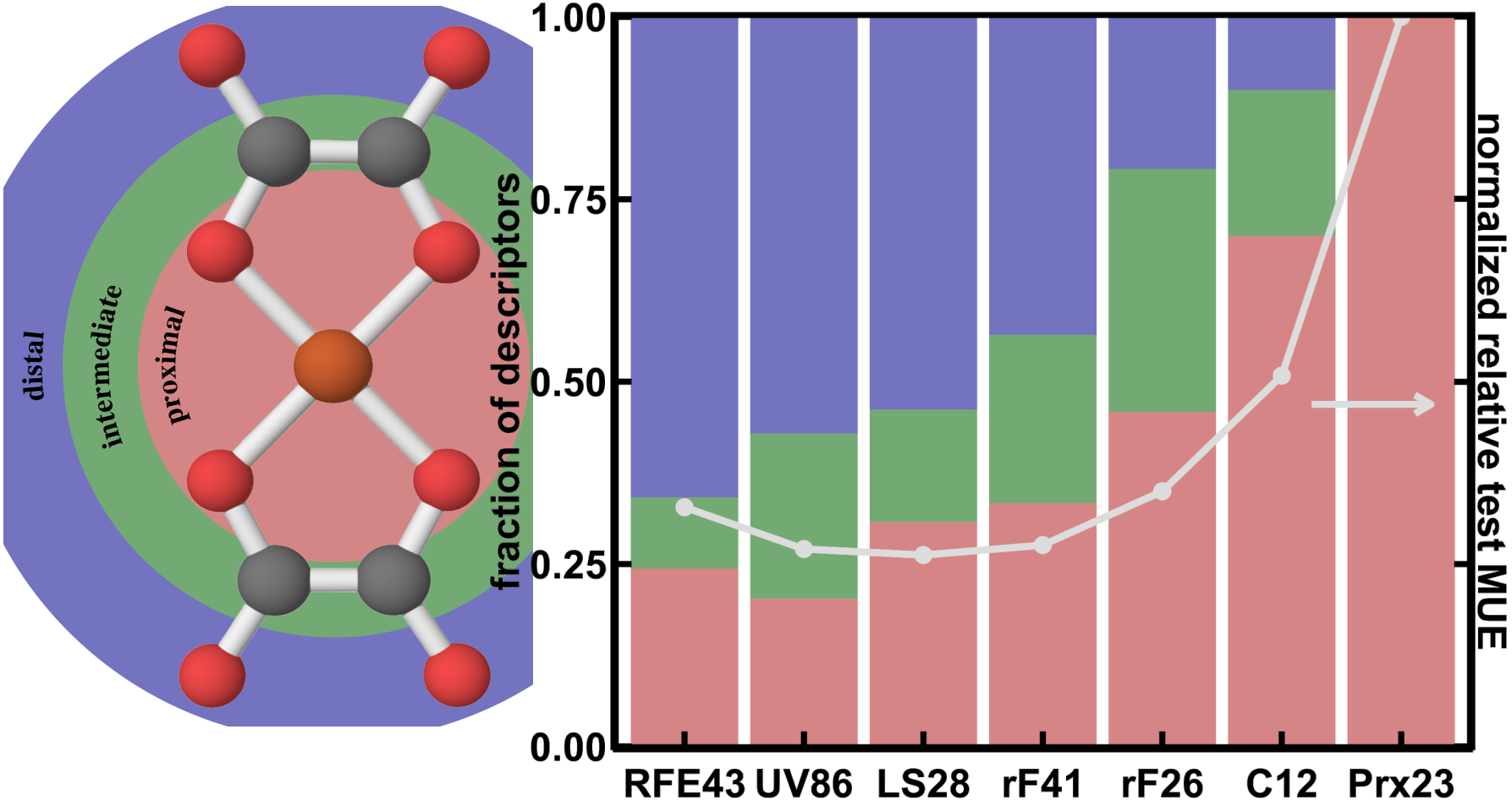
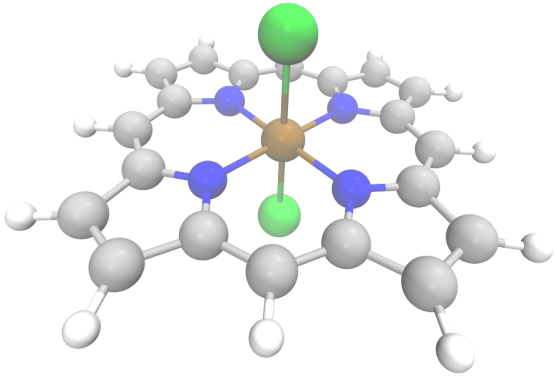


Janet, J.P., and Kulik, H.J., *arXiv*, 1708.06017, 2017.

Do features depend on properties?



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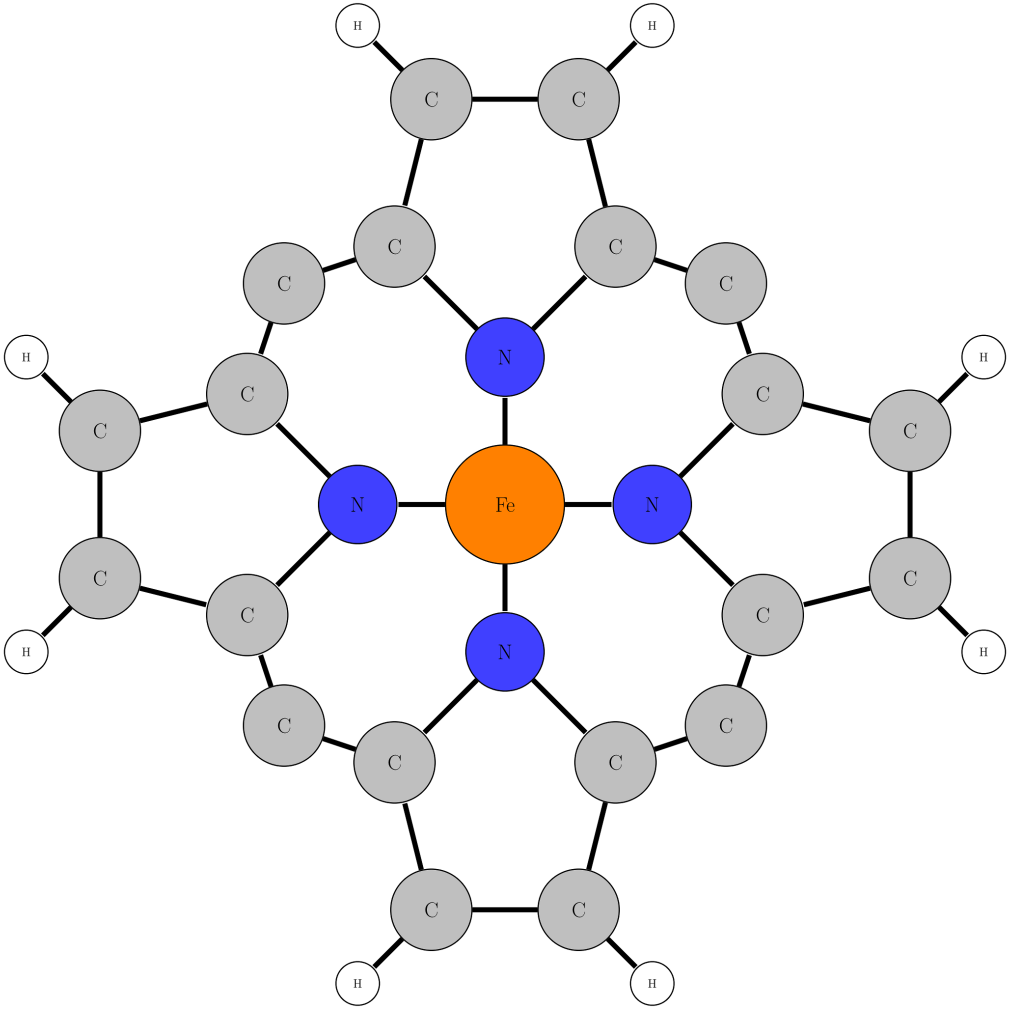
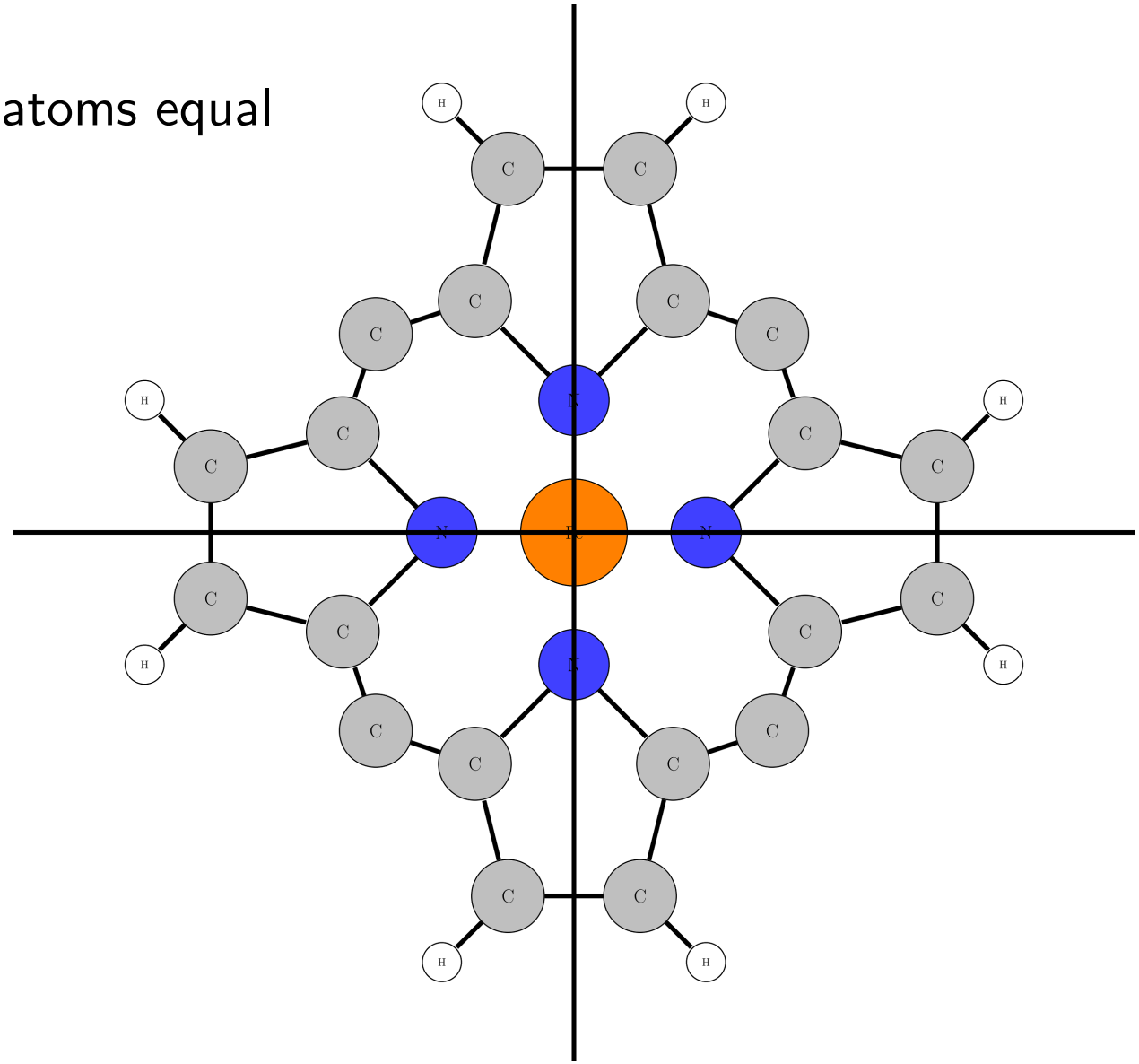


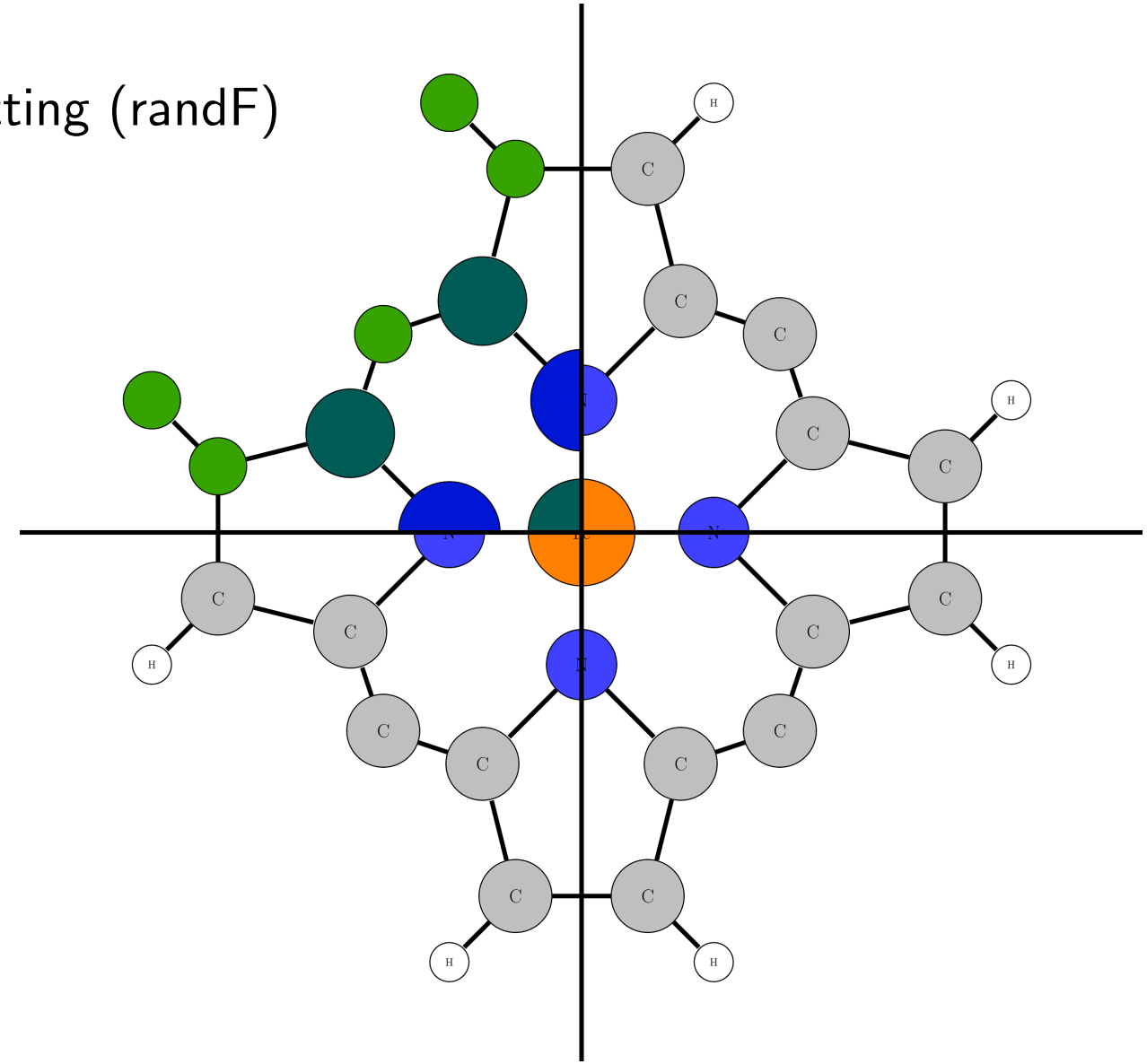
Do features depend on properties?

All atoms equal



Do features depend on properties?

spin splitting (randF)



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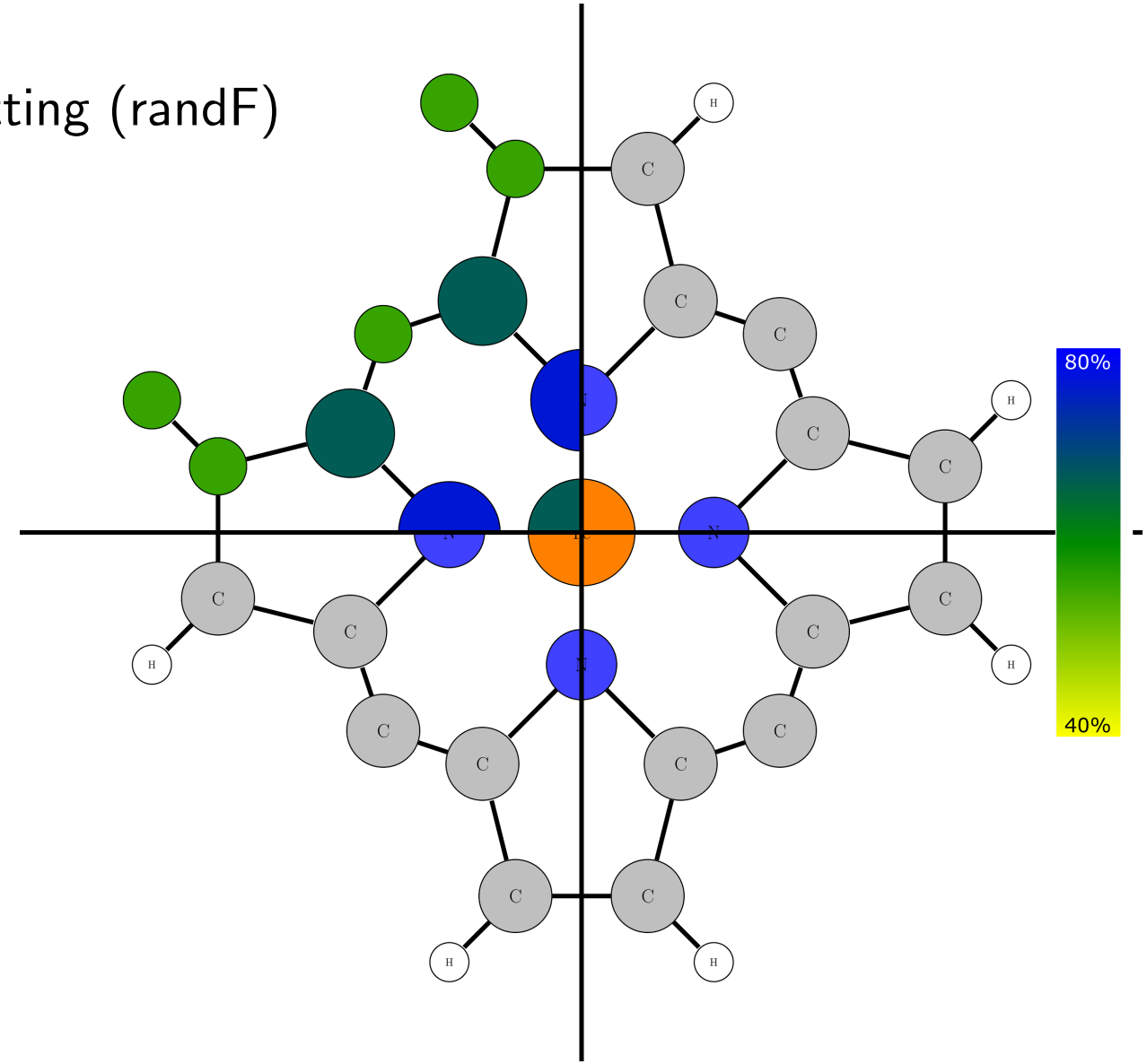

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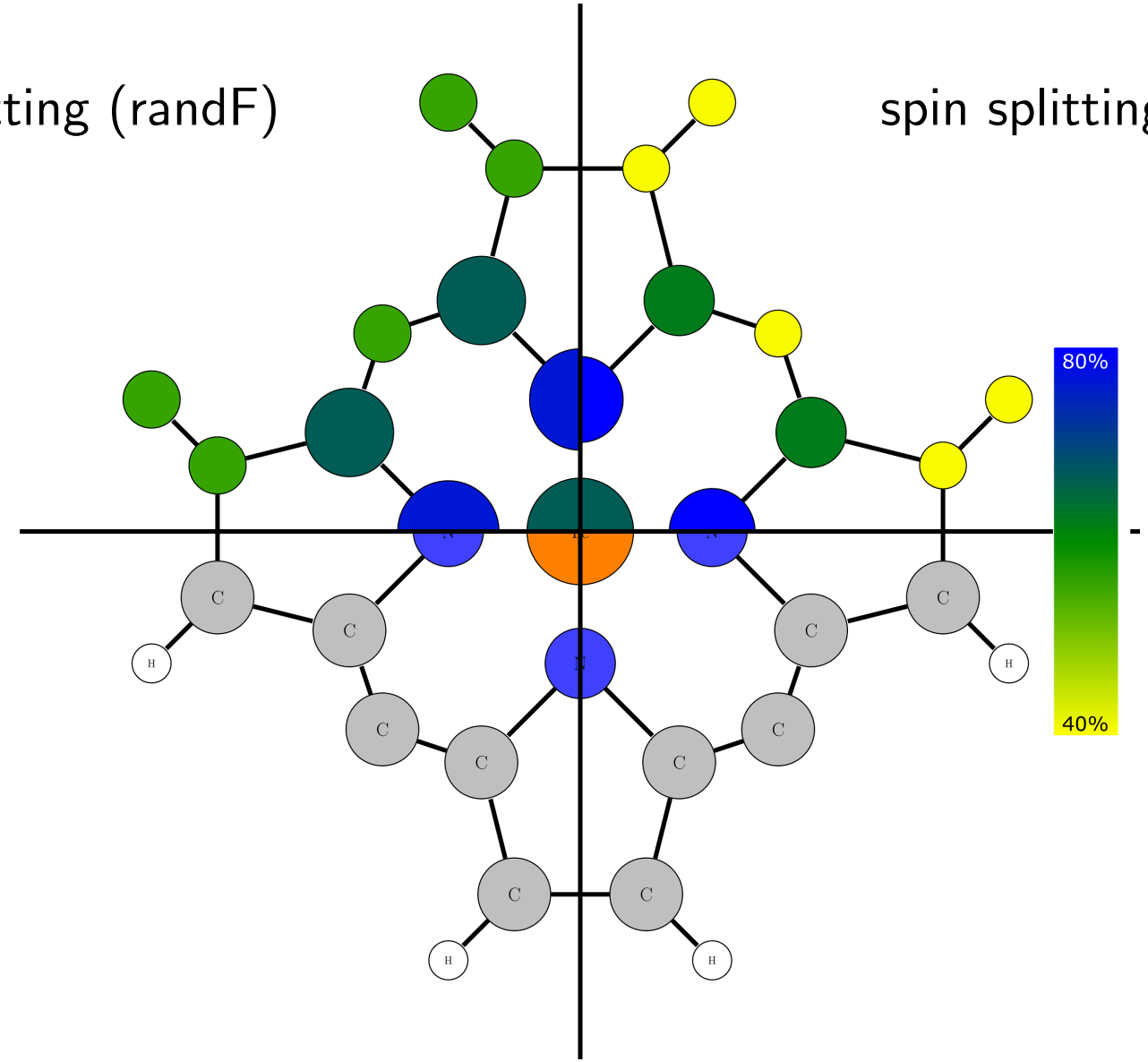

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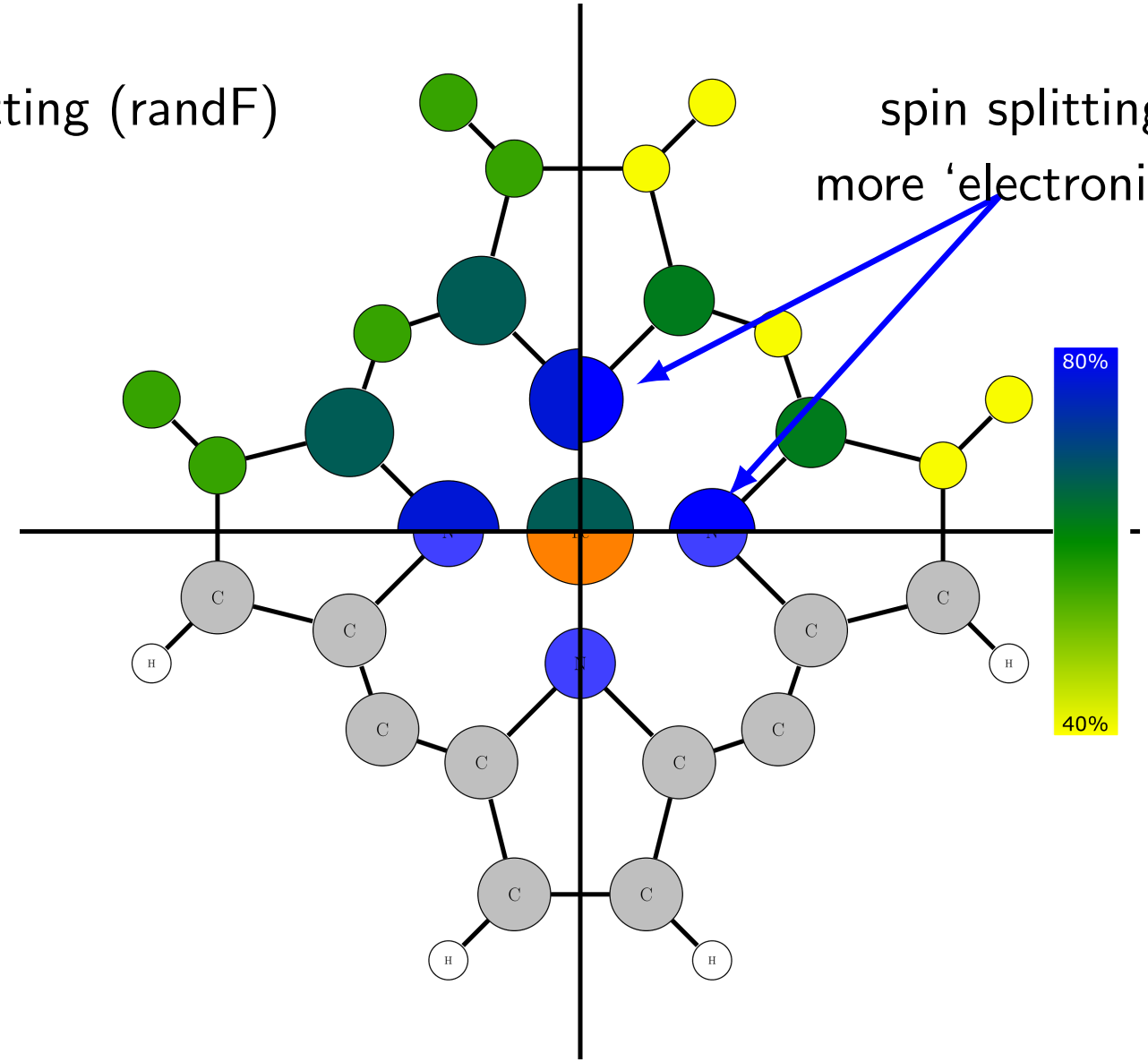
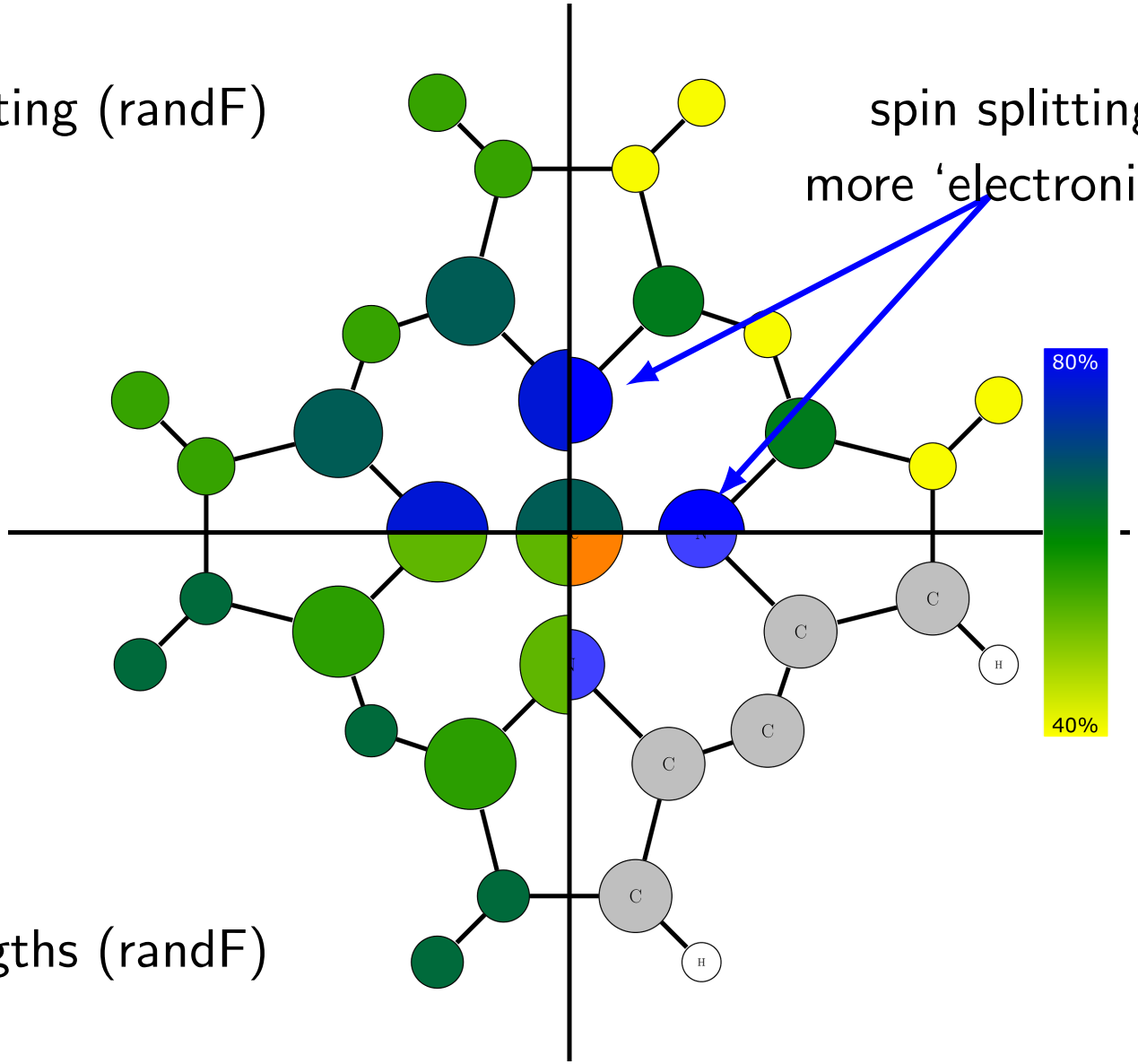


Do features depend on properties?

spin splitting (randF)

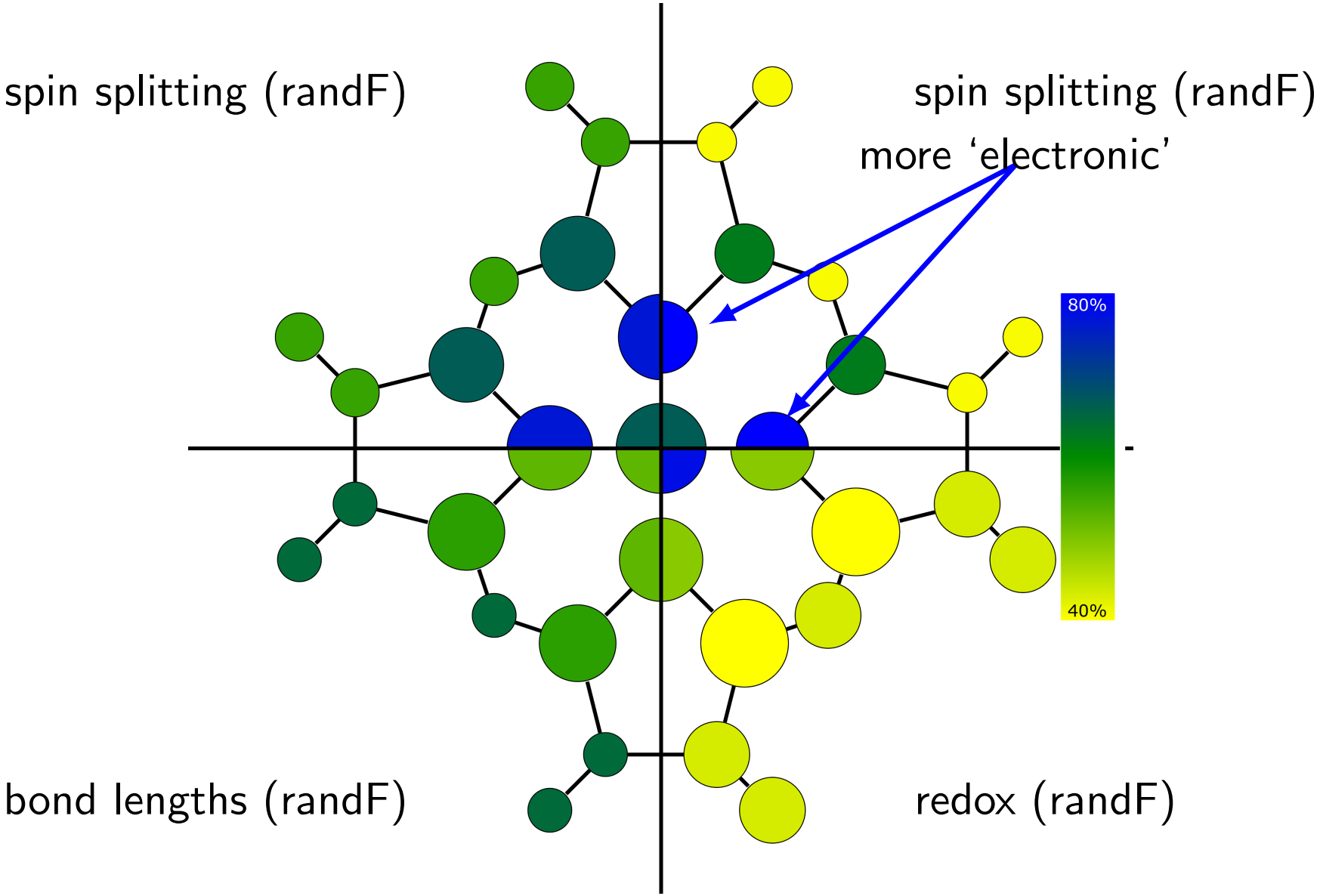
spin splitting (randF)

more 'electronic'

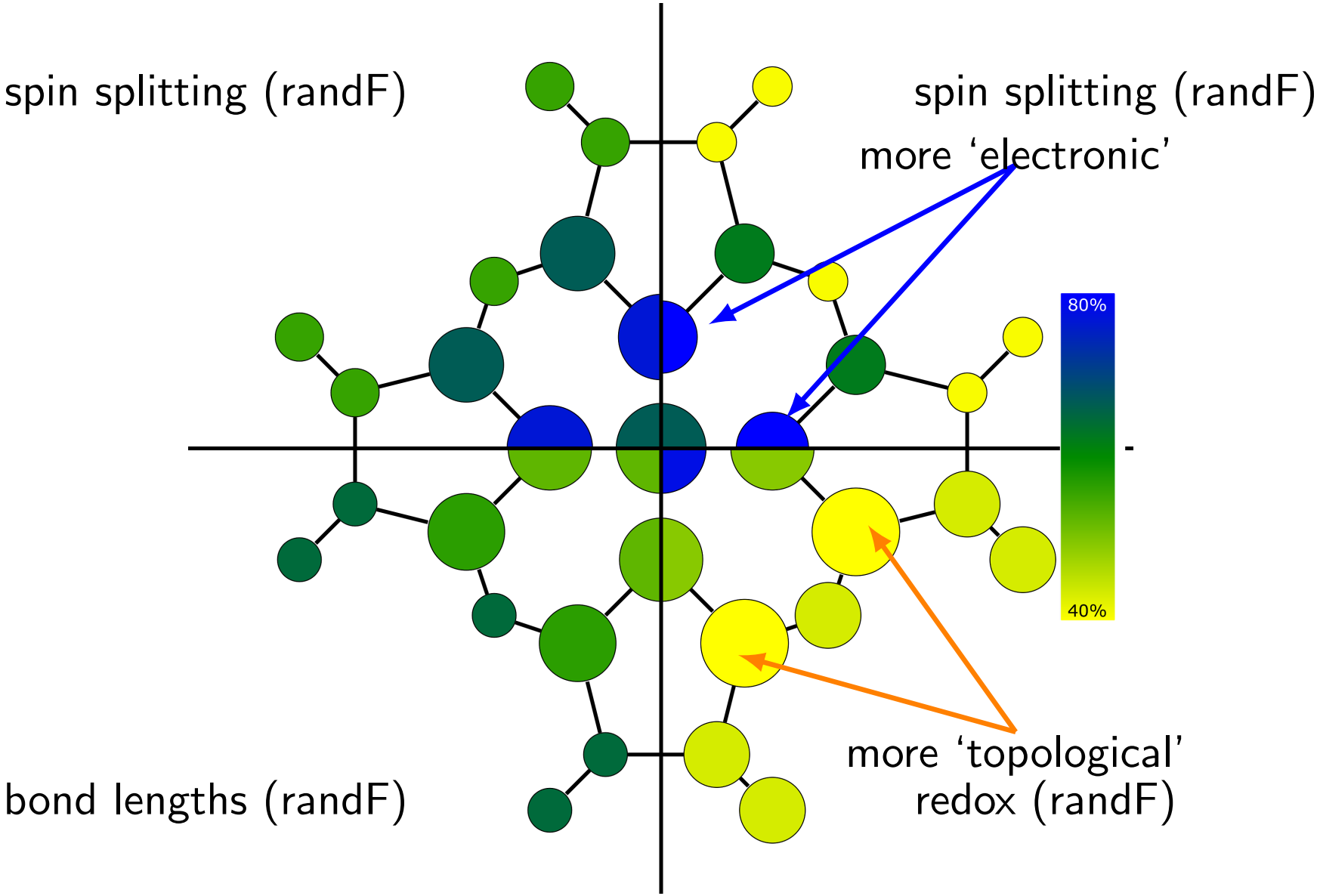


bond lengths (randF)

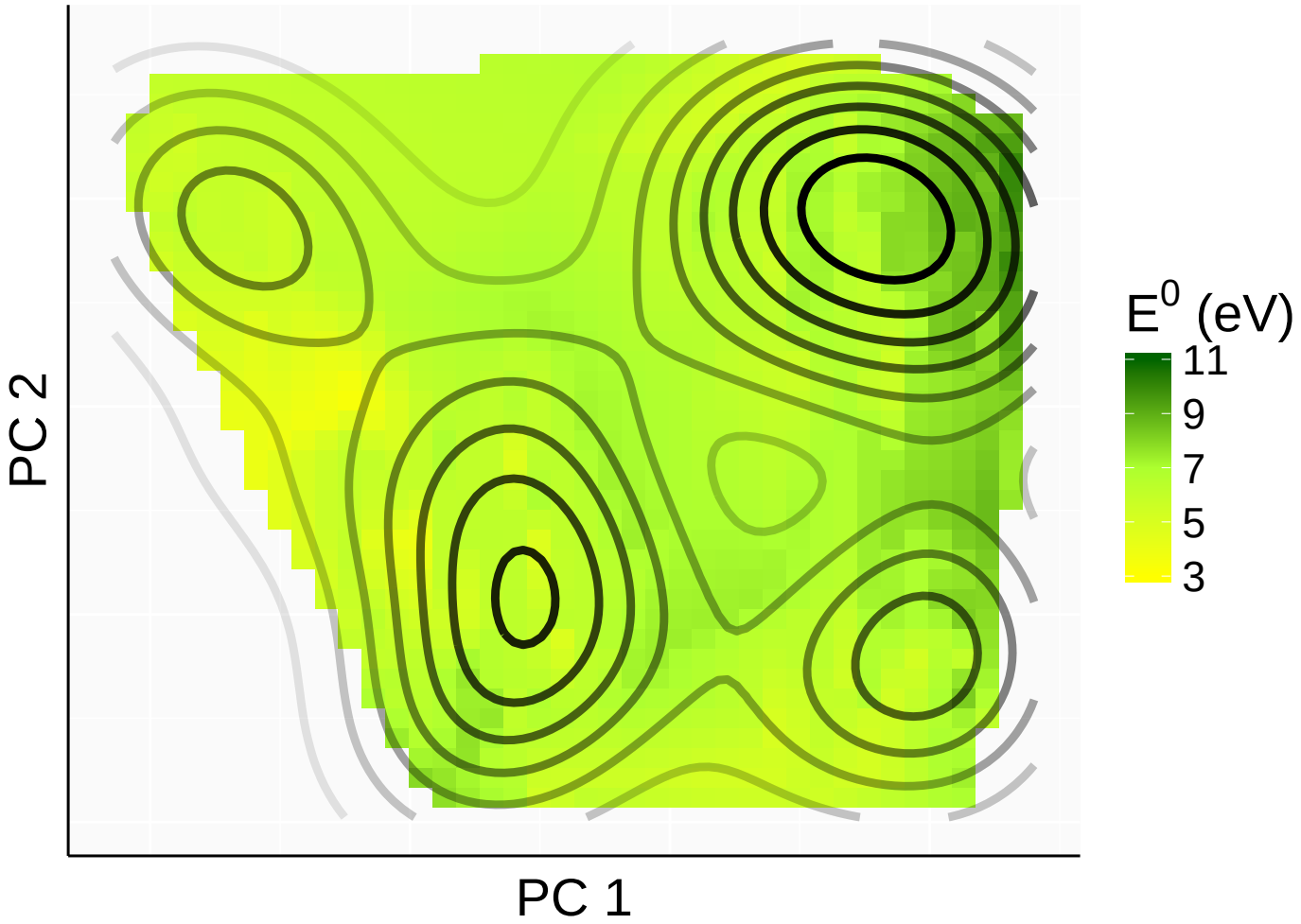
Do features depend on properties?



Do features depend on properties?



Mapping TM complex space



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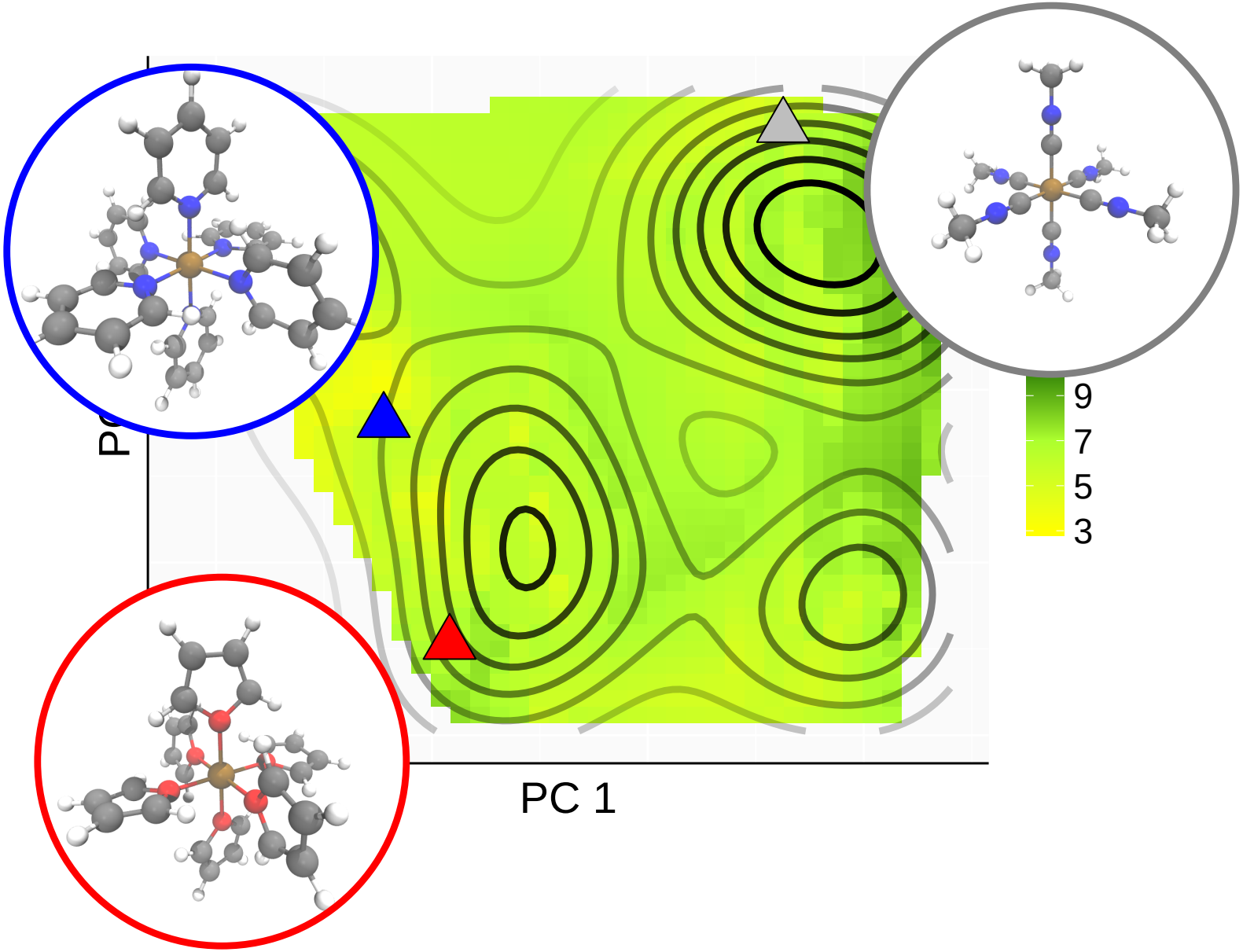

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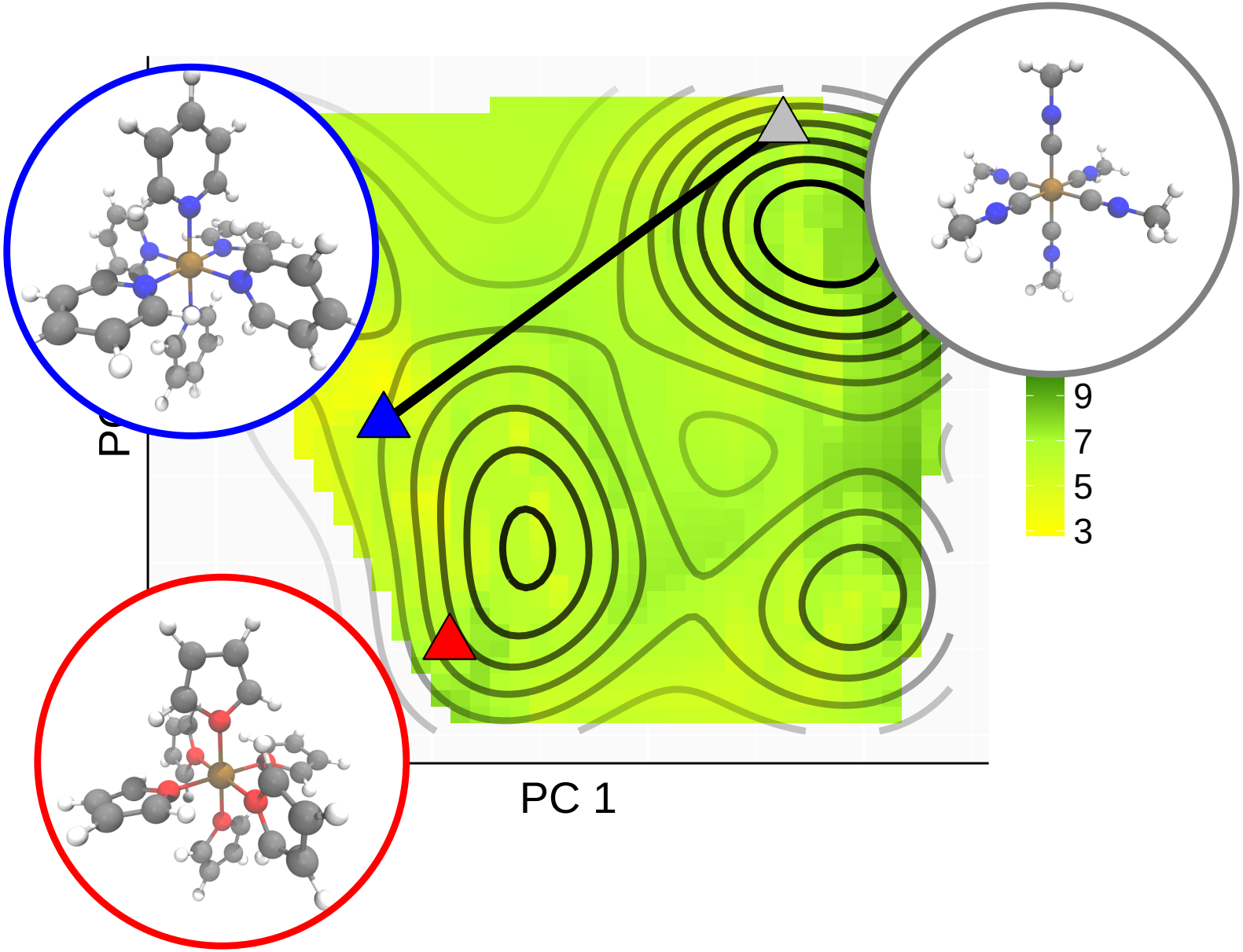
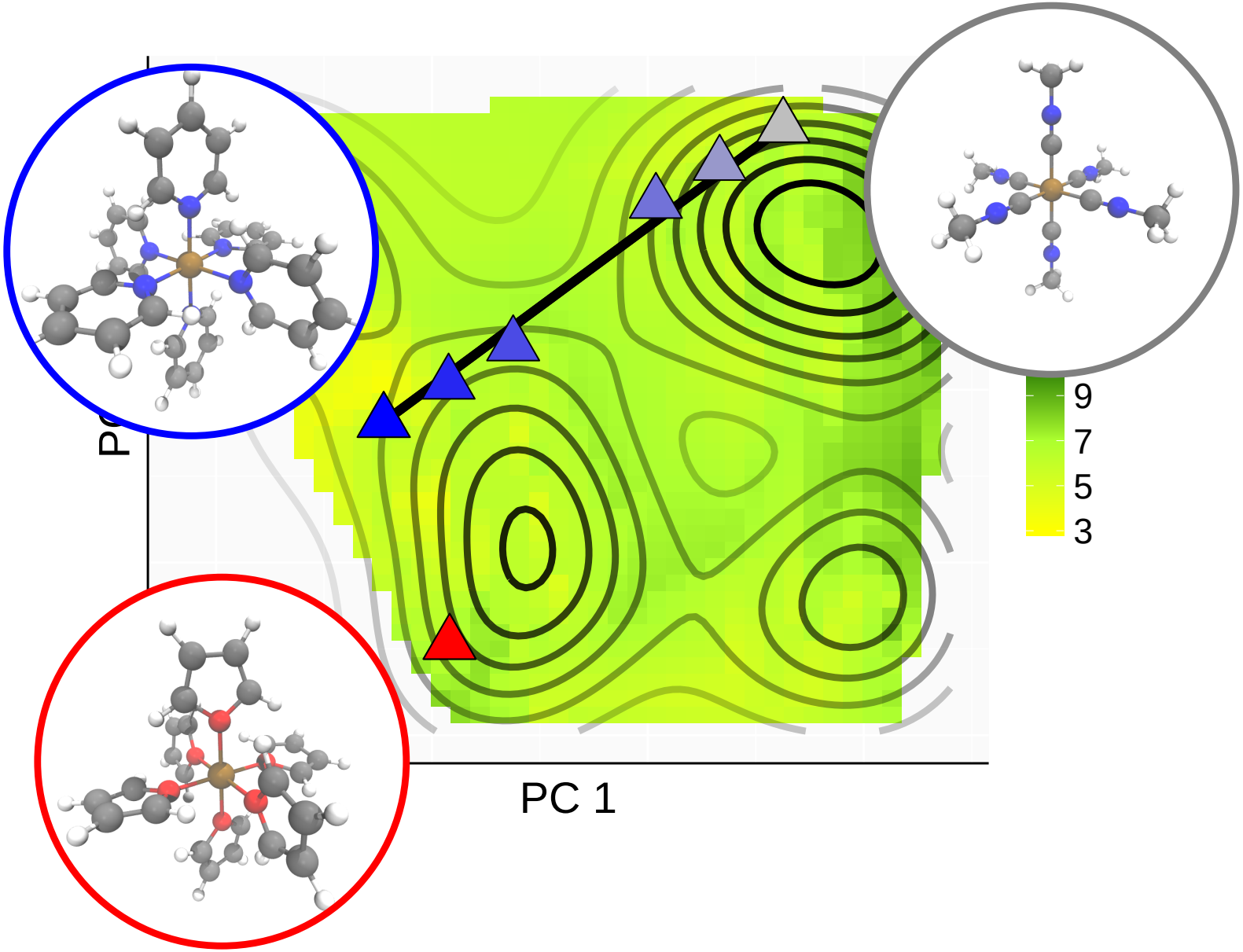
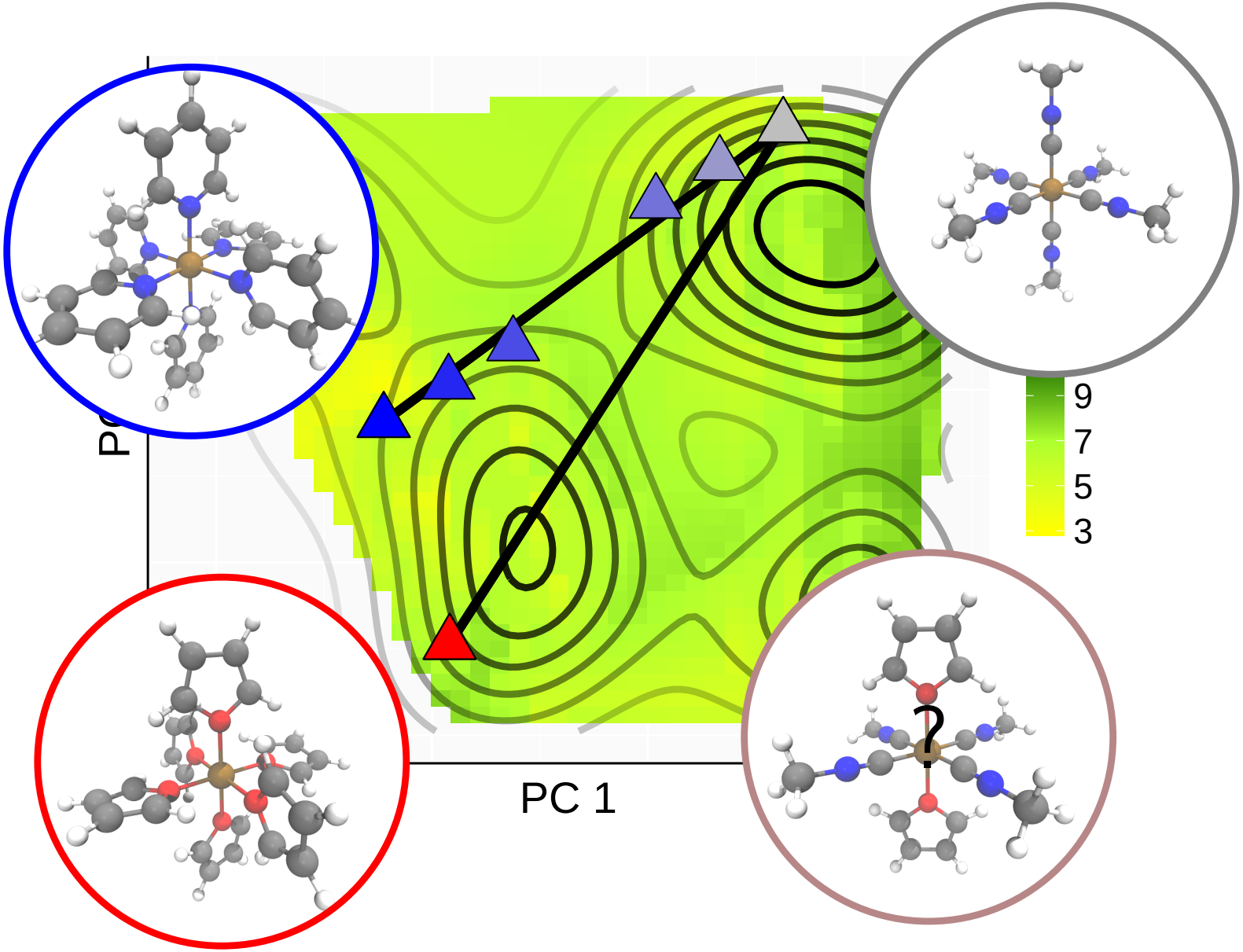


Mapping TM complex space



Mapping TM complex space



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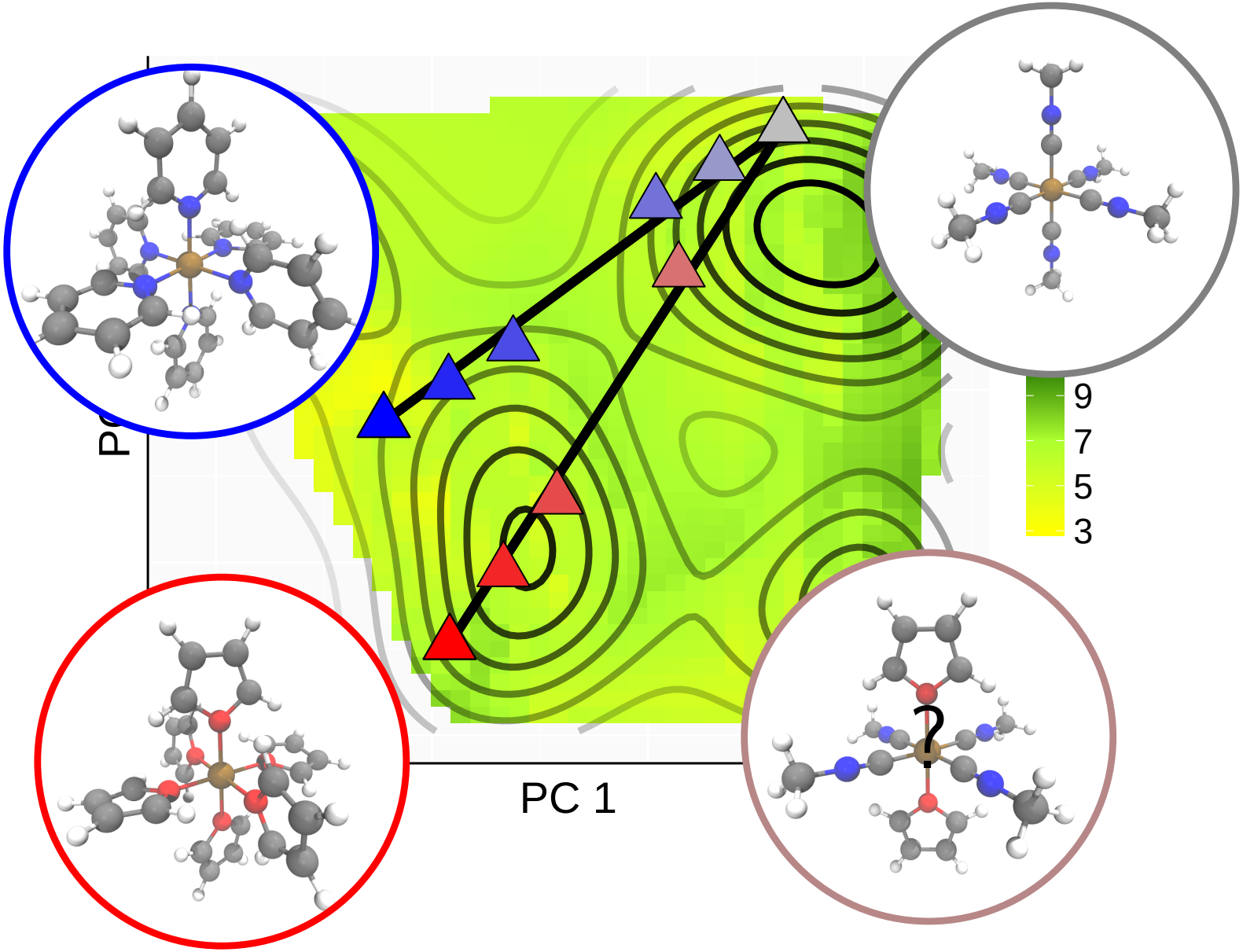
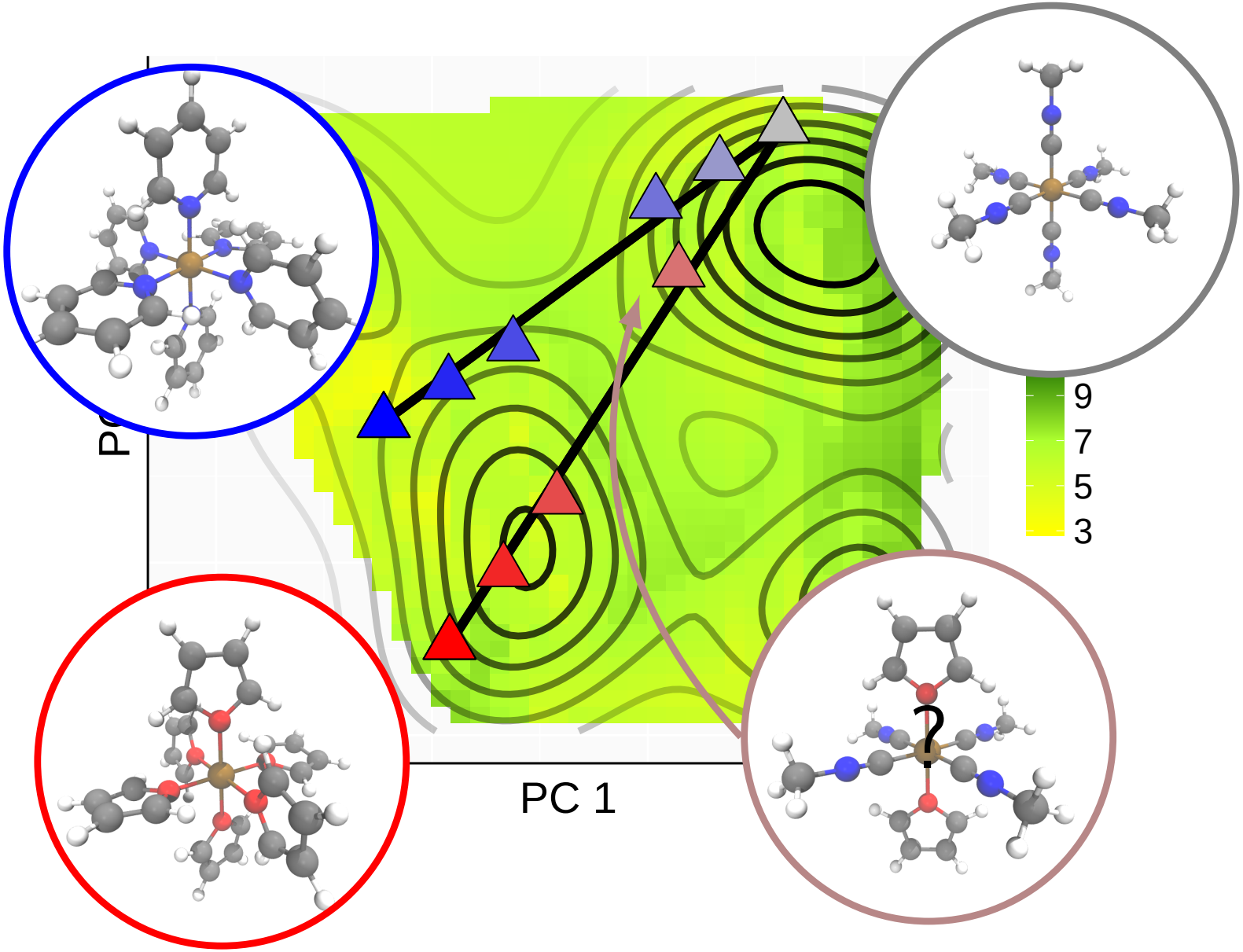


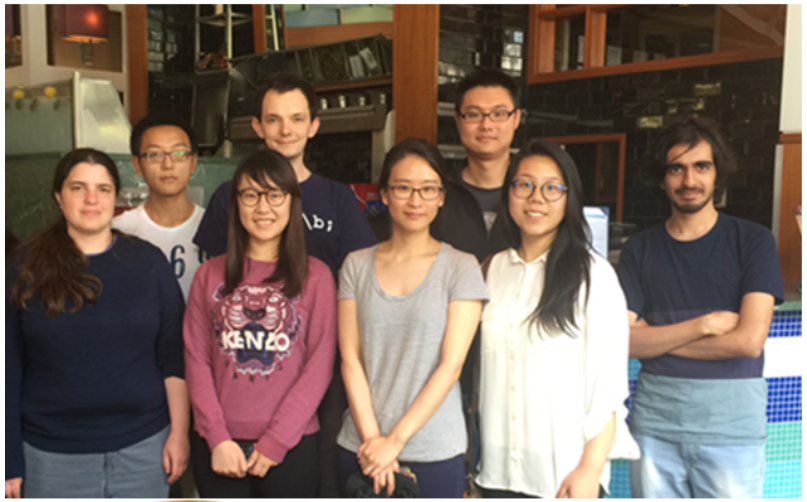
Mapping TM complex space



Acknowledgments

Conclusions:

- machine learning TM complexes faces unique challenges
- ACs are a promising starting point for low-cost descriptors
- different target properties depend on different physical variables and we can gain design insights but figuring out which



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