Chemically Transferable Potentials

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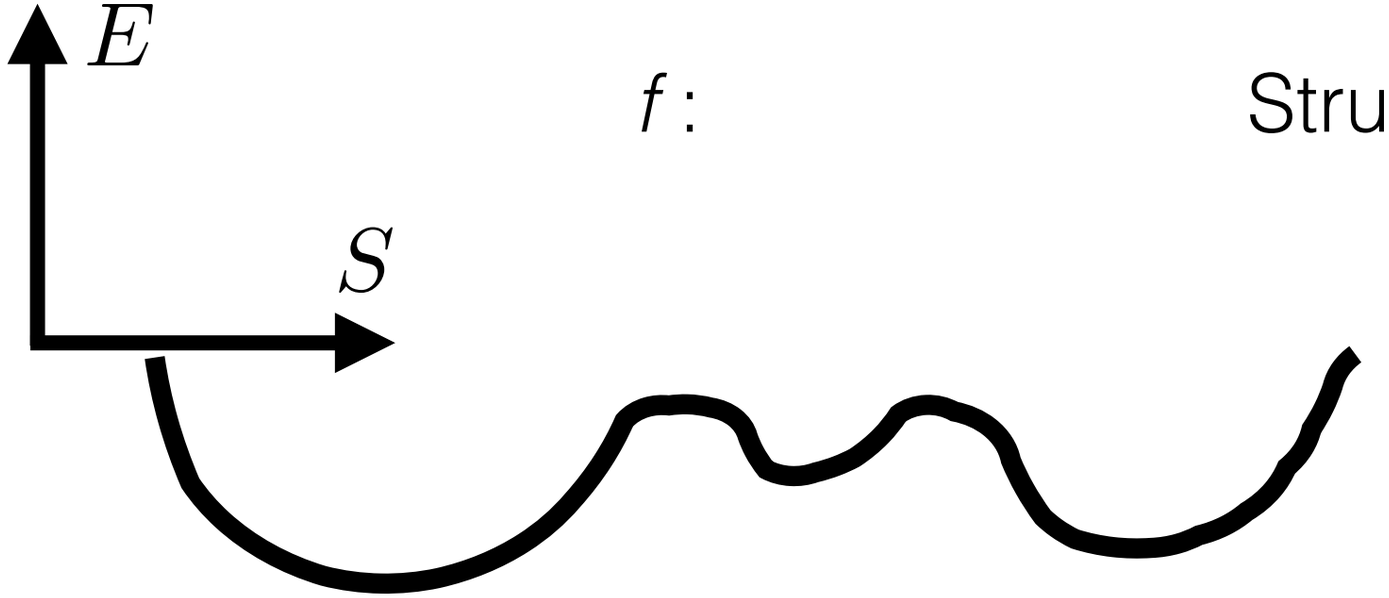

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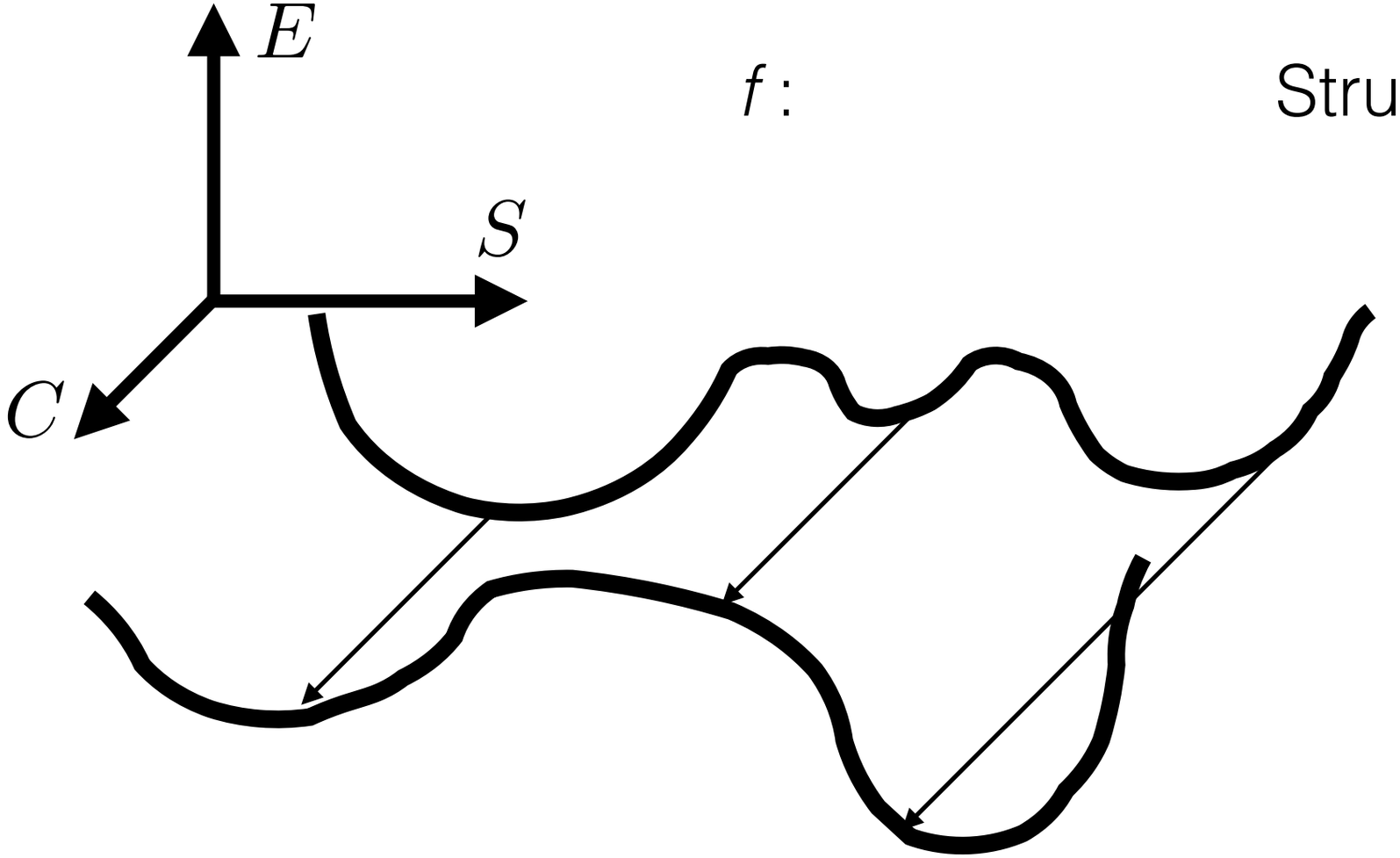

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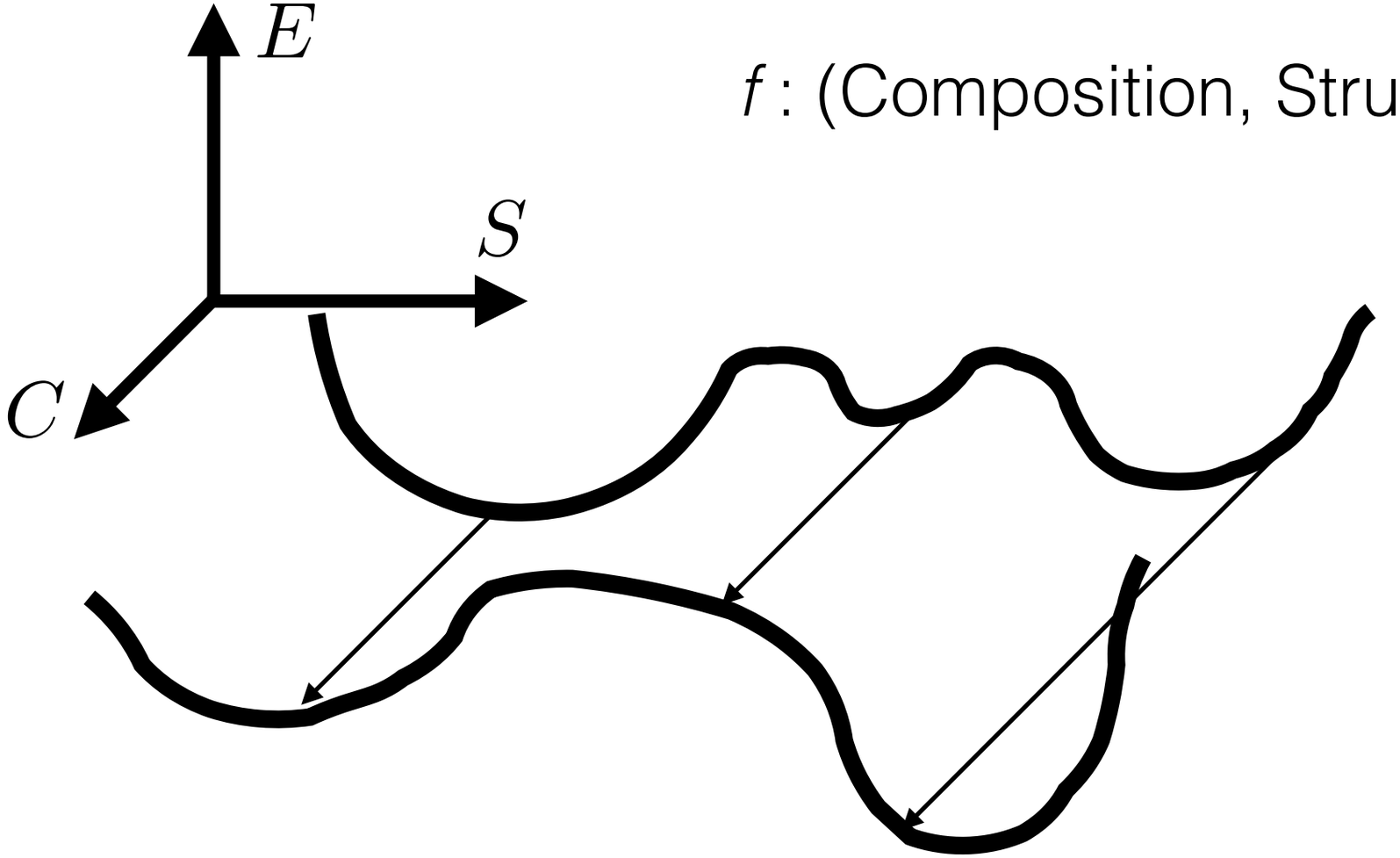

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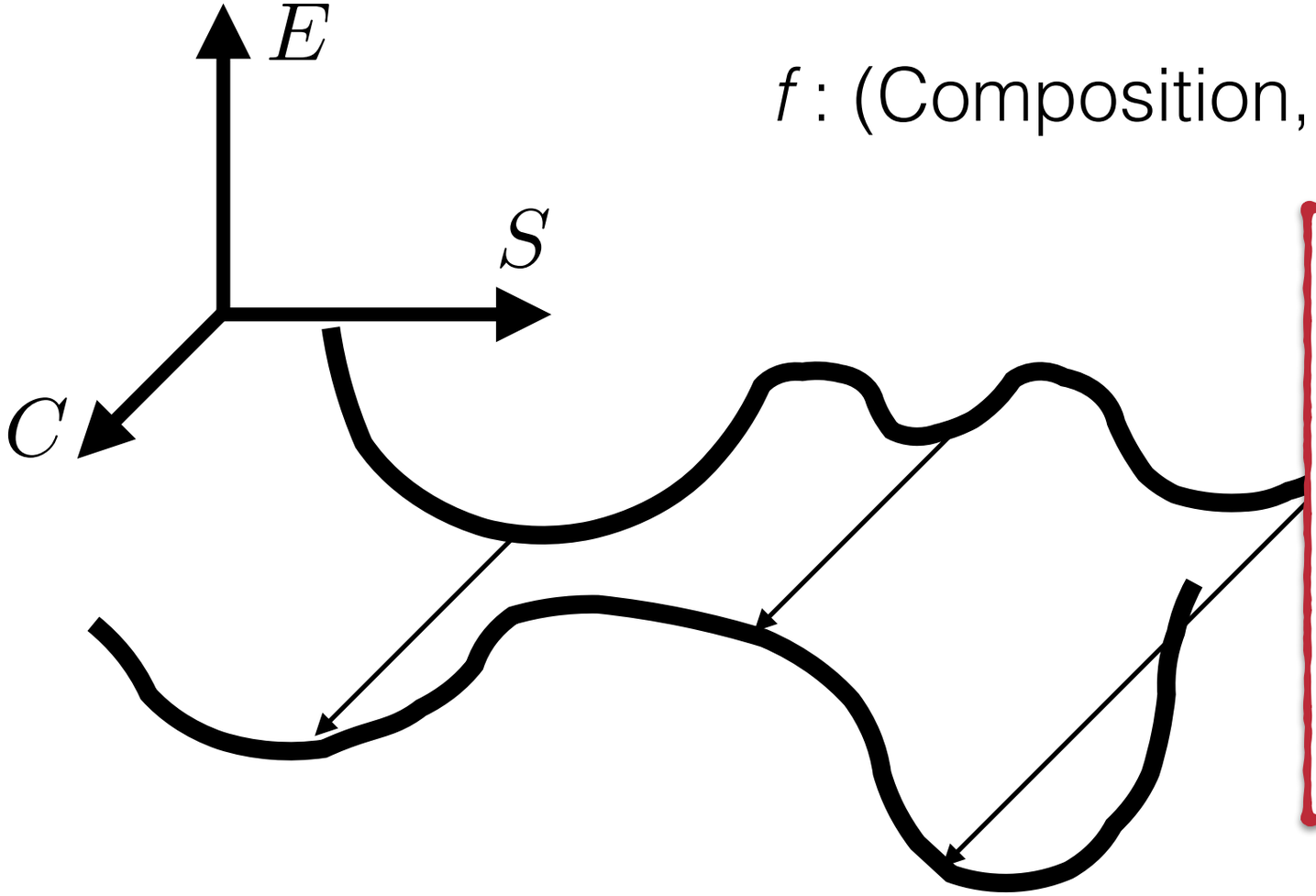
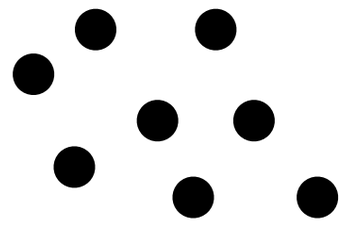


- prediction across chemical compound space
- improve PES fits by shared learning

Chemically transferable potentials

- start from simple potentials, e.g. 2-body potentials

$$E_{\mathrm{tot}} = \sum_{i \in \mathrm{pairs}} E_{2b}(r_i)$$



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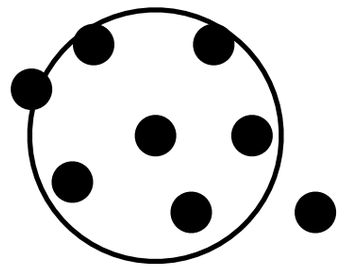

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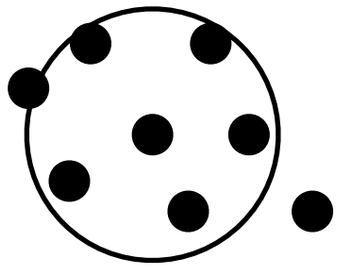

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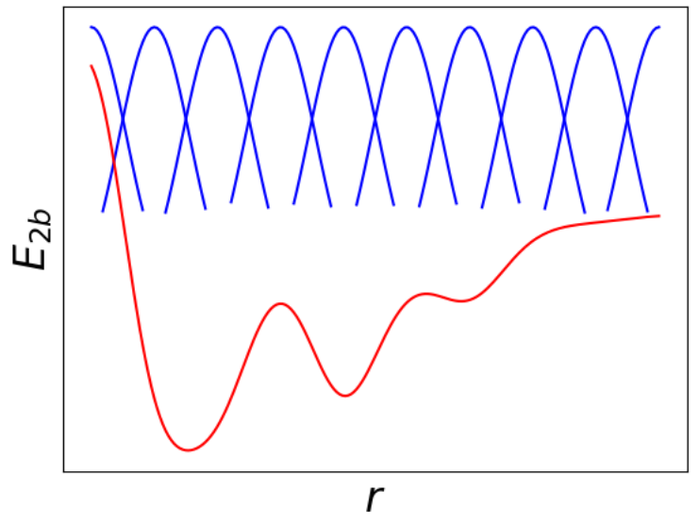

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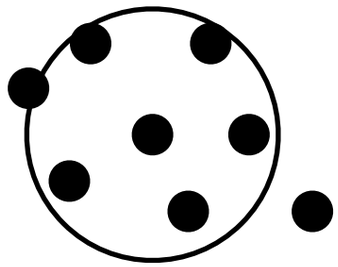

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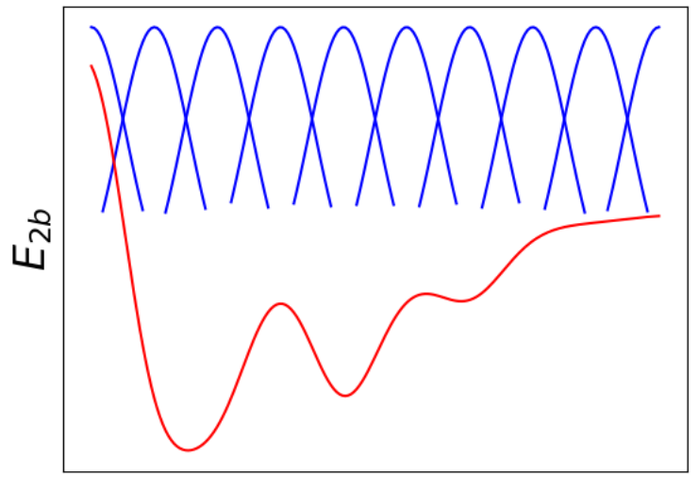

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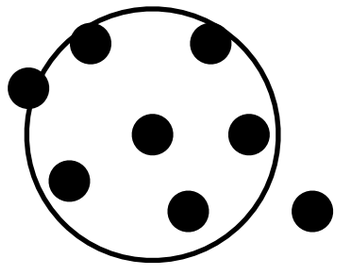

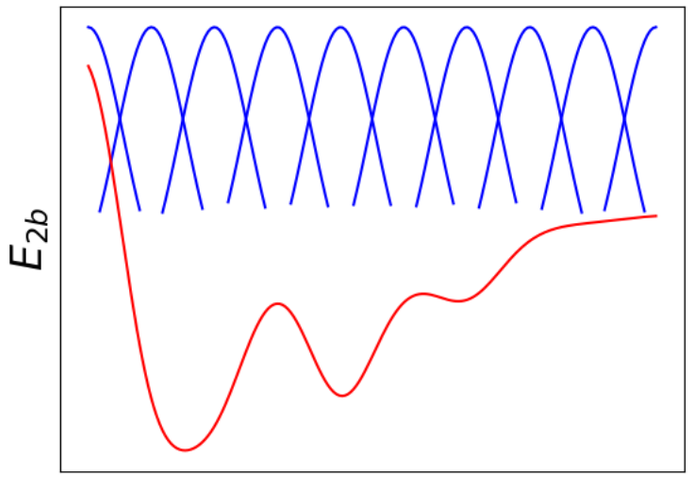

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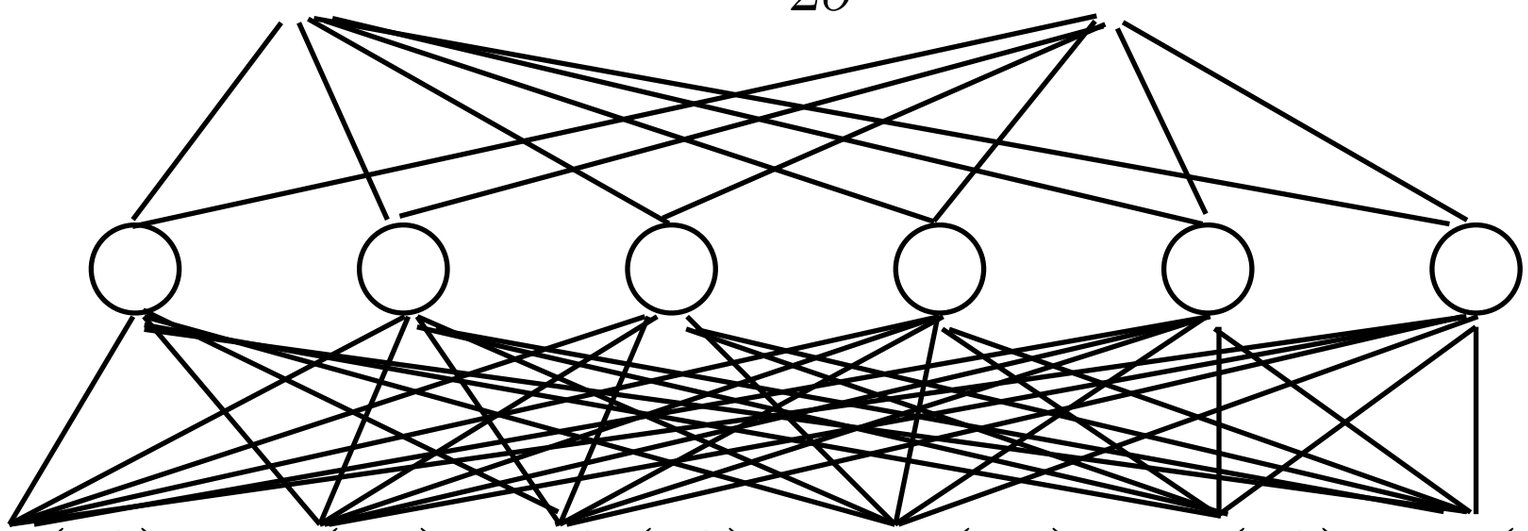

Results for 2b-potential and octet binaries

1885 data points = 82 compounds x 4 phases x 5/8 volumes

Input features: $\mathrm{IP}, \quad \mathrm{EA}, \quad r_s, \quad n_{\mathrm{valence}}$

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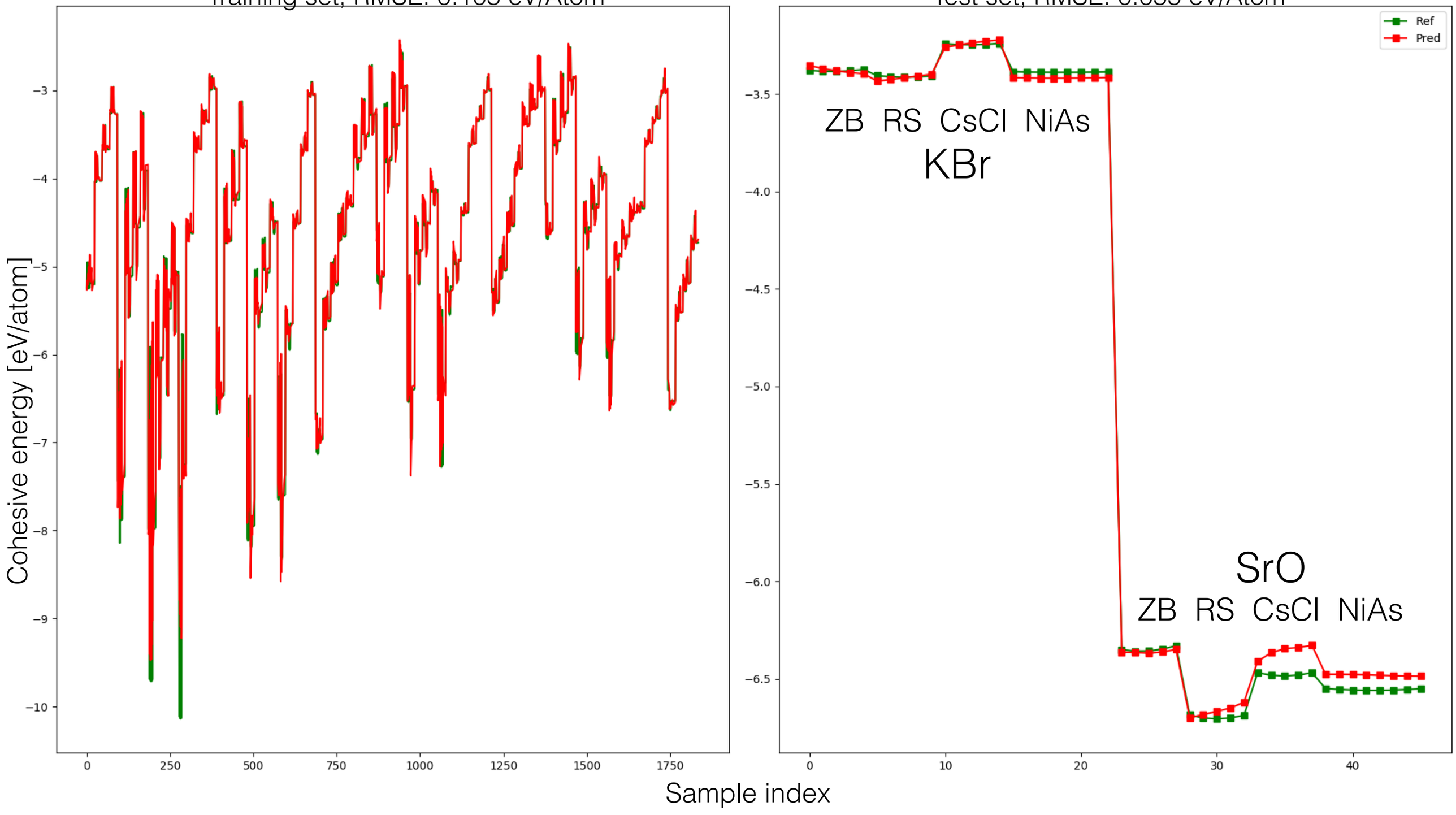
Training set, RMSE: 0.105 eV/Atom

Test set, RMSE: 0.055 eV/Atom



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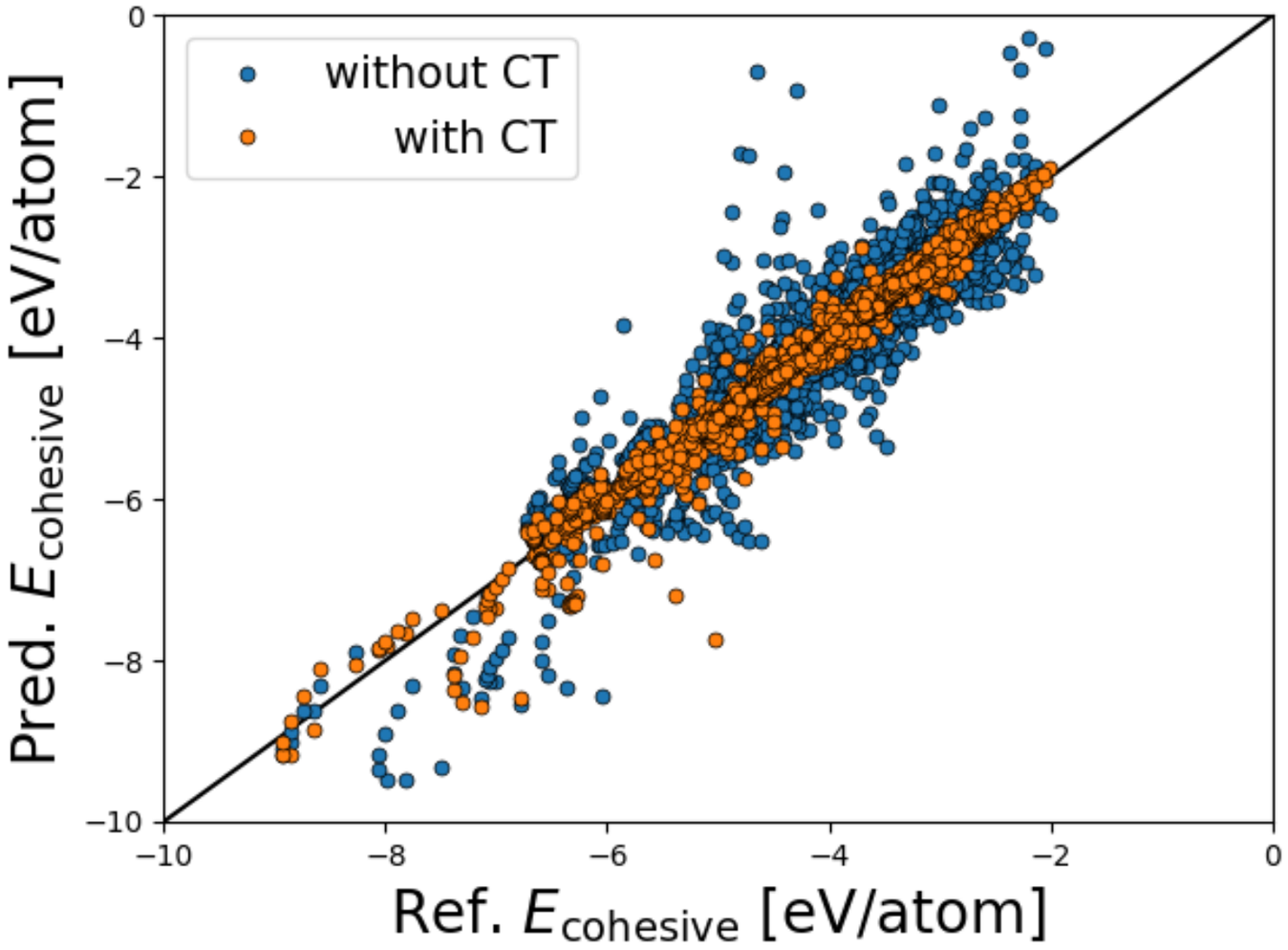

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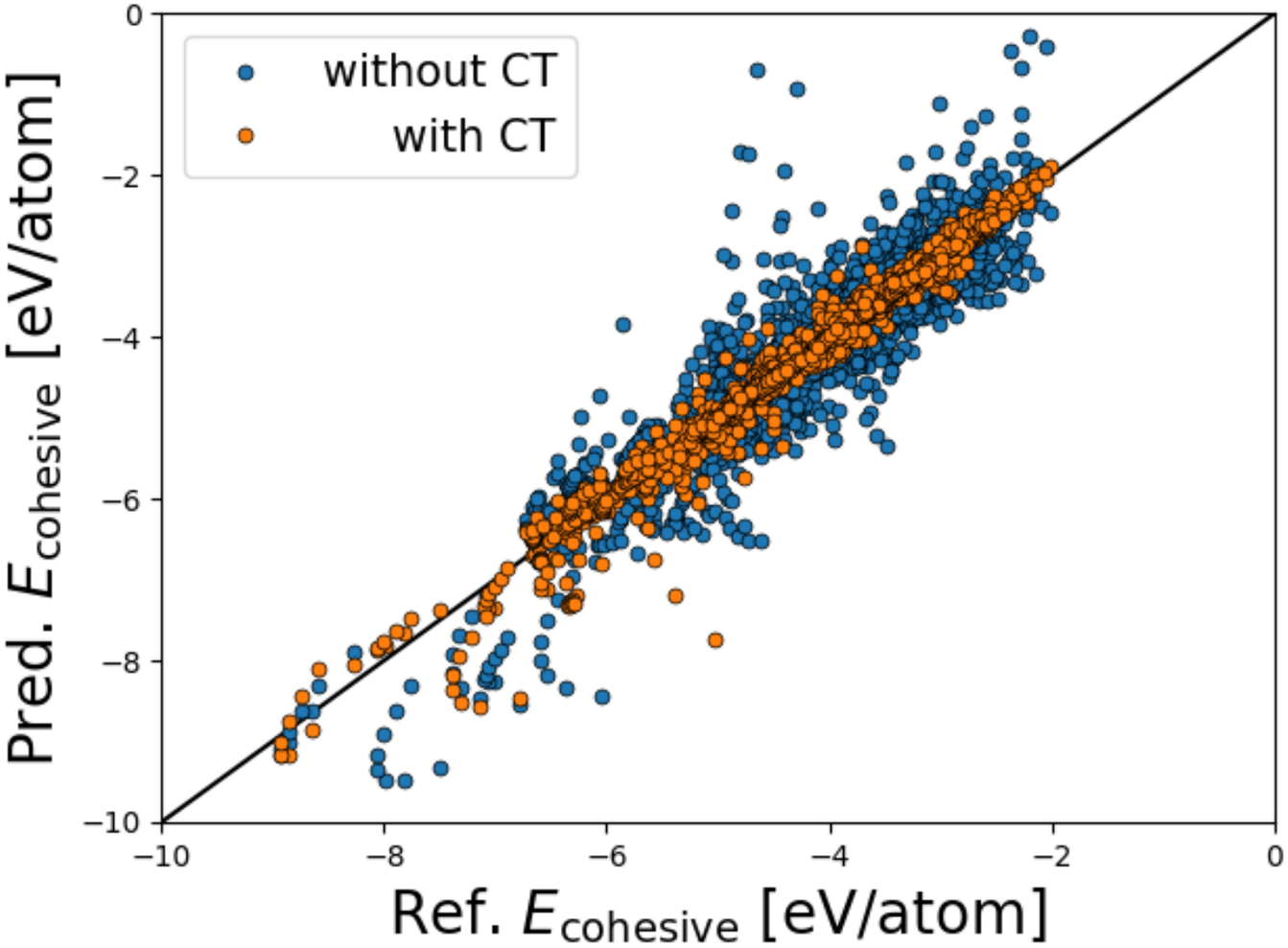

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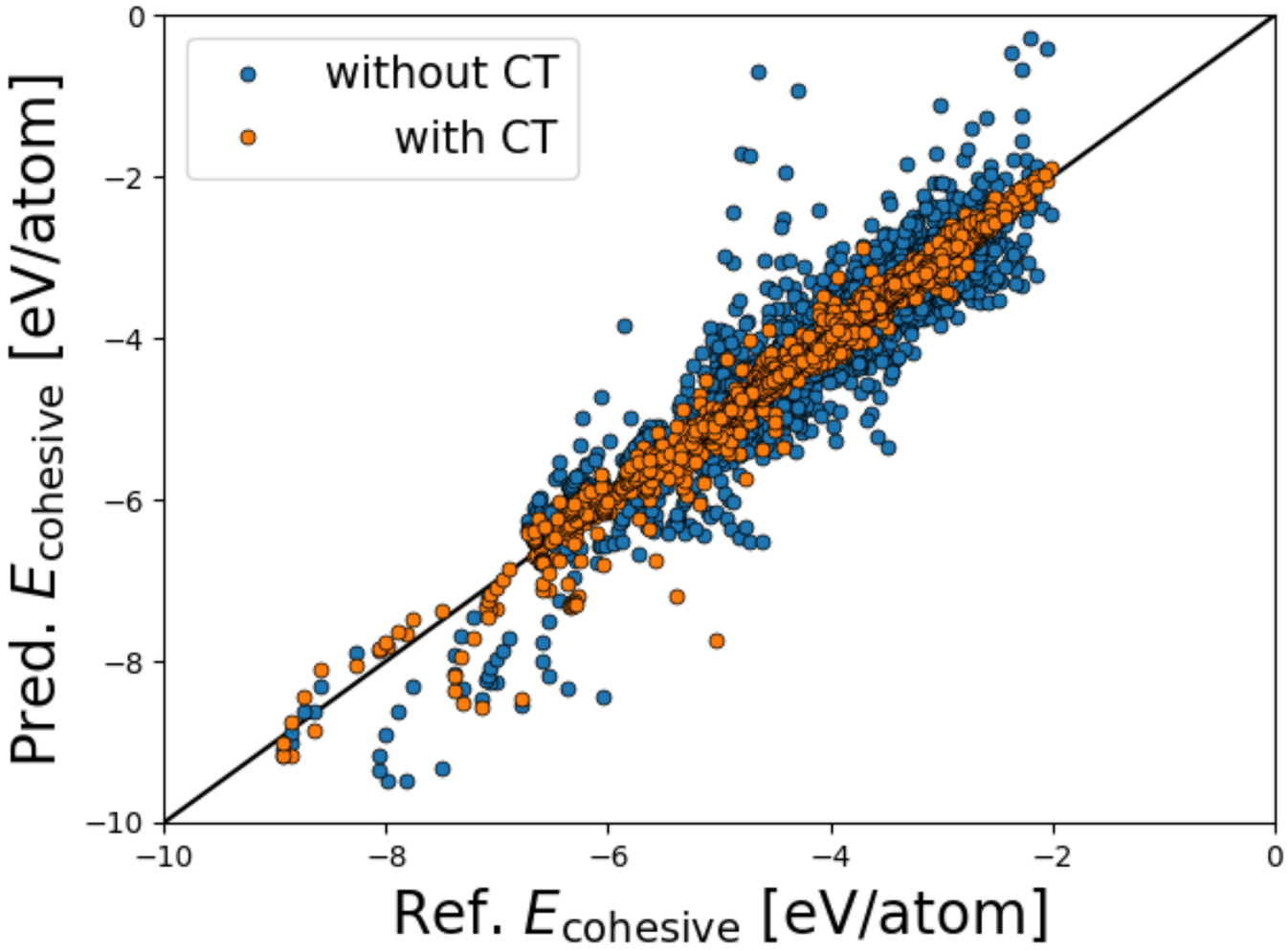

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The CT approach regularizes the ML potential parameters using physics

Summary

- New idea on how to transfer potentials across compound space
- Chemically transferred potentials regularize the the machine learning potentials

2b-potential fit to Stillinger-Weber potential