



University of
Dayton

Intelligent Algorithms for the Optimization of Rare-Earth Cation Forcefield Parameters

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Introduction

Rare Earth Elements

The periodic table shows the following elements highlighted as Rare Earth Elements:

- Lanthanides (Green):** La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb.
- Actinides (Yellow):** Ac, Th, Pa, U, Np, Pu, Am, Cm, Bk, Cf, Es, Fm, Md, No.

- Bottom row – Useful in both civilian and military life.
- High-end electronics, research, etc.
- Extremely difficult to extract
- Cannot be accurately modeled due to missing/inaccurate parameters

Bayesian Optimization

- Machine-learning algorithm
- Can optimize without needing to know the function it is optimizing
- Optimizes in parallel – Fast and allows for multiple elements to be optimized at once

Objectives:

- Utilize HFE and IOD calculations to find forcefield parameters
- Utilize machine-learning optimization algorithm for easy and efficient discovery of forcefield parameters

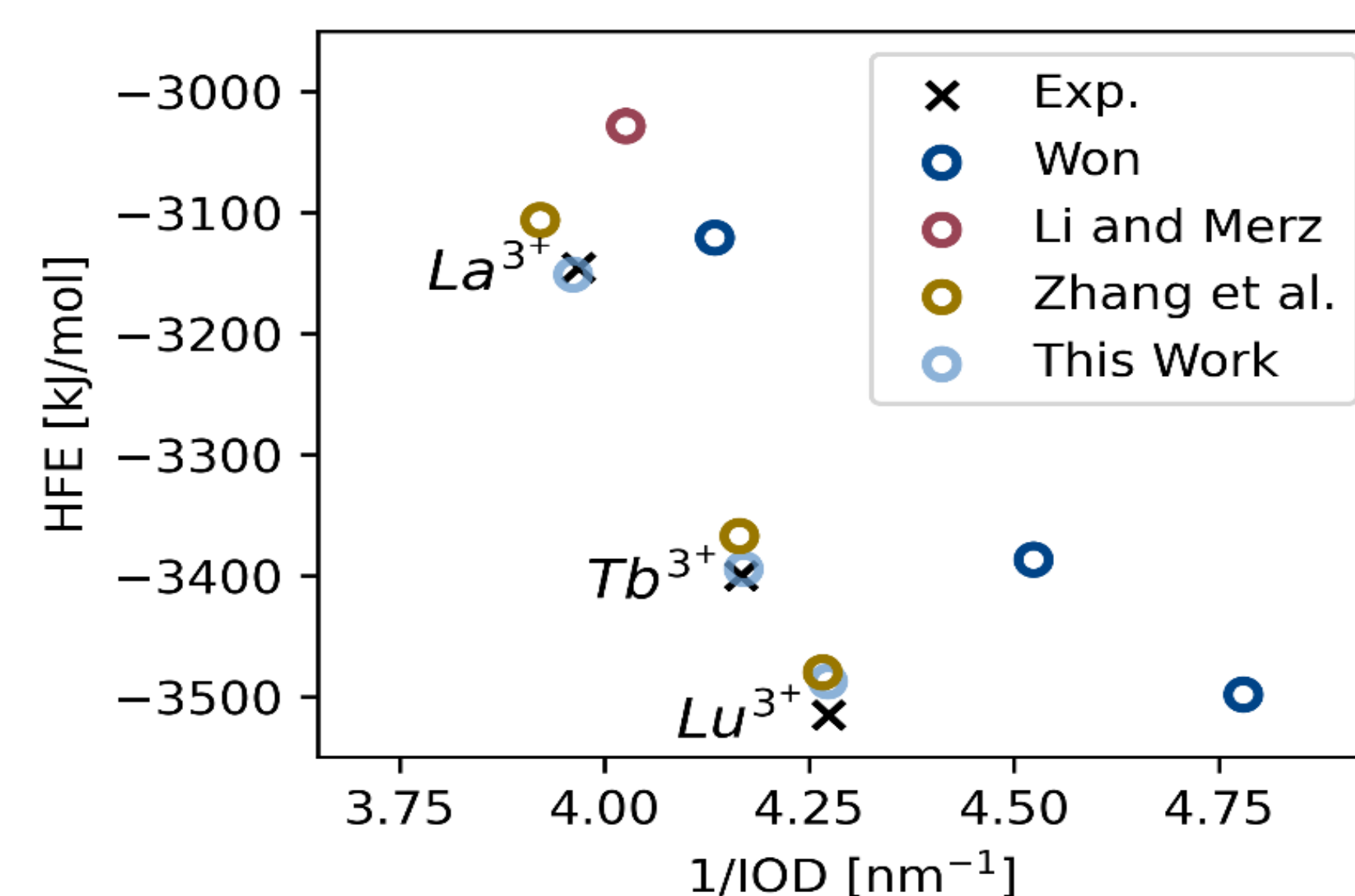
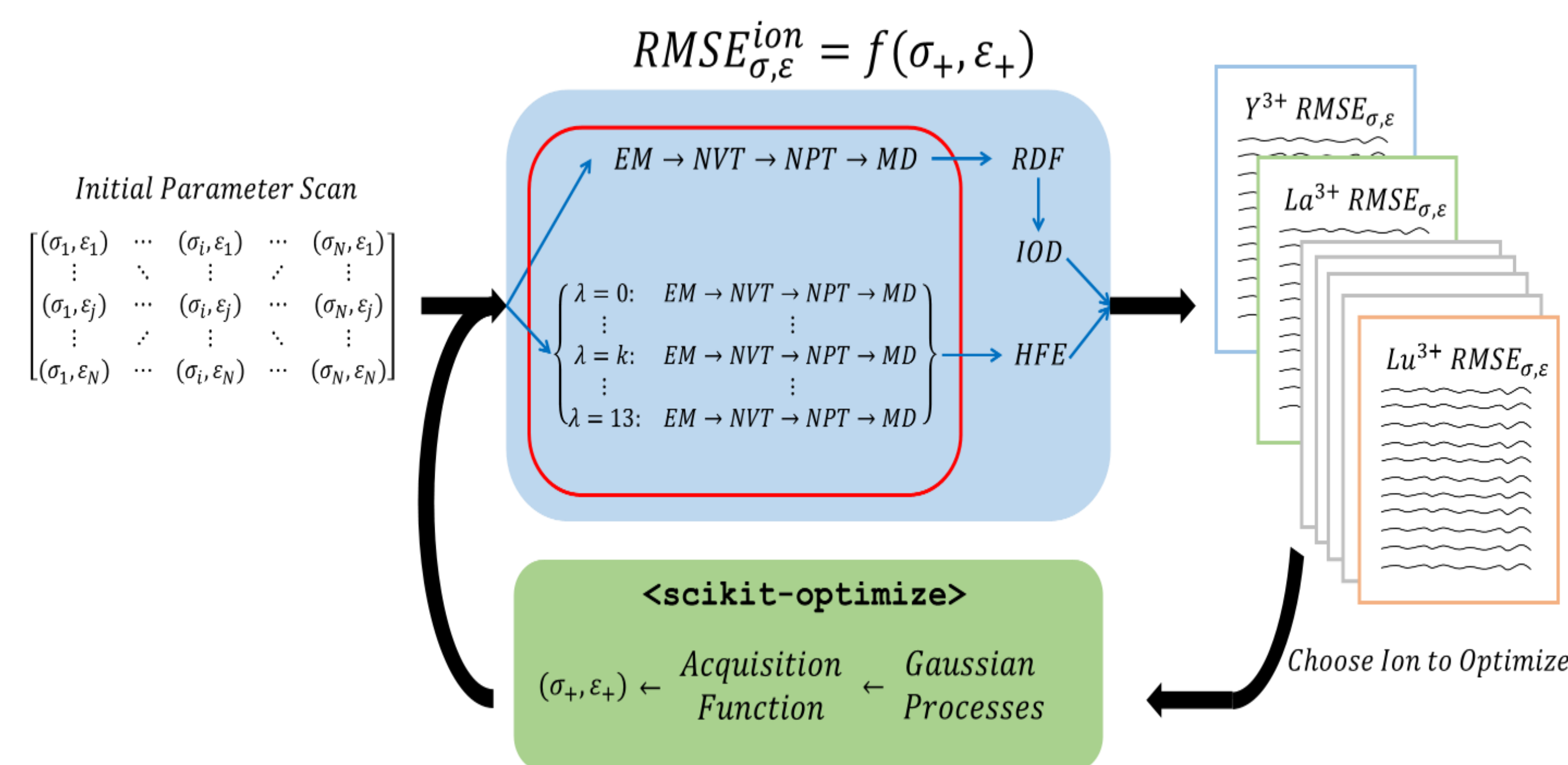
Approach

Hydration Free Energy (HFE) and Ion-Oxygen Distance (IOD)

- HFE: Energy released when ions undergo hydration
- IOD: Positive cation “pulls” and flips negative oxygens towards it
- Both simple and calculated from forcefield parameters

Optimization Algorithm

- Utilized parallel Bayesian optimization to decrease computational time needed, and Python to automate the process



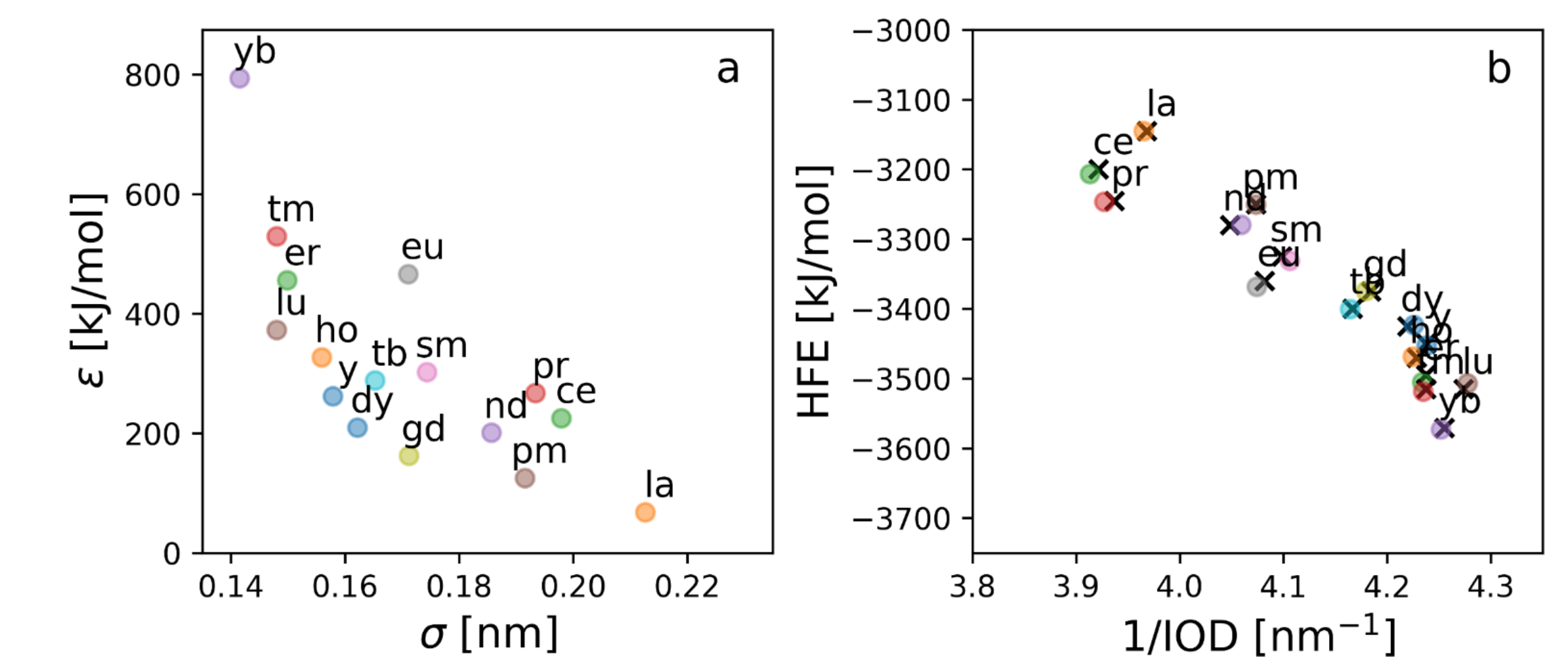
- Extremely accurate results in less than 7 runs

- **Goal:** Reduce root mean squared error to < 10%

Results

Table 1: Sample results

REE	σ (nm)	ϵ (kJ/mol)	HFE (kJ/mol)	IOD (nm)	RMSE %
La	0.245	13.6	-3195	0.252	1.12
Tb	0.195	52.3	-3402	0.241	0.29
Lu	0.171	103.8	-3515	0.236	0.56



Conclusions/ Future Directions

- Automation proved invaluable to the discovery process
- Cross parameters are valid for water – Will need corrections for protein binding
- End Goal: Utilize the results discovered here on further MD simulations on protein binding (Biomining)

Acknowledgements



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