Intelligent Algorithms for the Optimization of Rare Earth Cation Force Field Parameters

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Research Interests

- Molecular dynamics simulations and HPC data analysis
- Machine learning algorithms and automation

Technical Expertise

- GROMACS Experience
- Linux Experience
- HPC Experience

Hobbies

- Music
- Hiking
- Boating
- Stargazing

Education

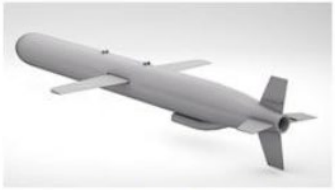
- Bachelors of Chemical Engineering
- Pursuing Masters in Materials Engineering

Why Rare Earth Elements?

Many Defense Systems Relies on REEs

Predator Drone
Neodymium, Samarium
Electric Motors and Guidance

Smart Bomb
Neodymium, Samarium
Electric Motors and Guidance



Tomahawk Cruise Missile
Neodymium, Samarium
Electric Motors and Guidance

Night Vision Goggles
Terbium, Erbium, Gadolinium
Optical Lenses

F-22 Fighter Jet
Europium, Yttrium Terbium, Erbium
Optical Systems, Visuals and Fiber Optics

Bullet Proof Vest
Yttrium
Hardened Ceramics

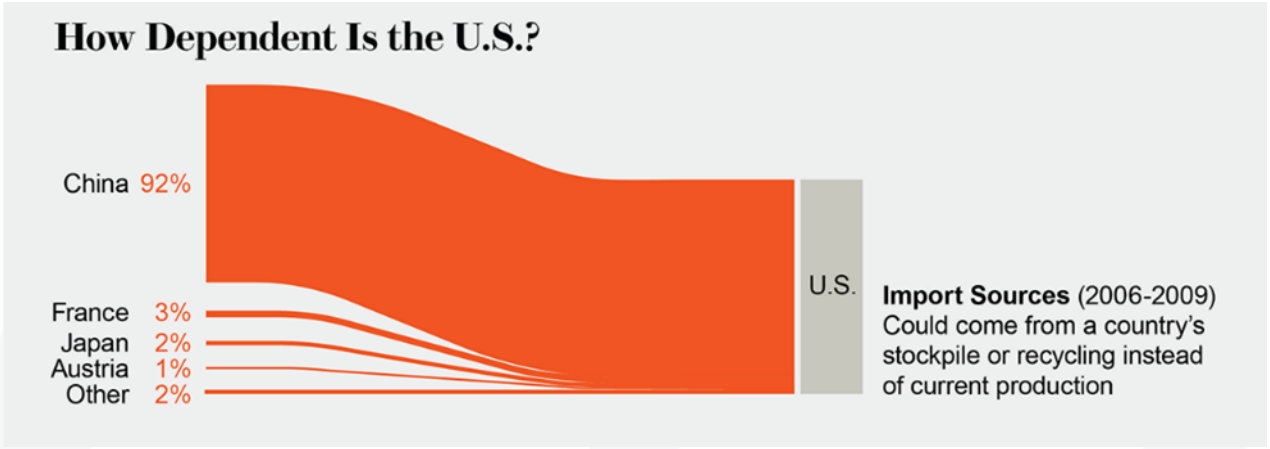
Bradley Tank
Yttrium
Hardened Ceramics

Radar Detection
Europium, Lutetium
Signal Amplification

Nuclear Submarine
Europium, Lutetium
Sonar Detection

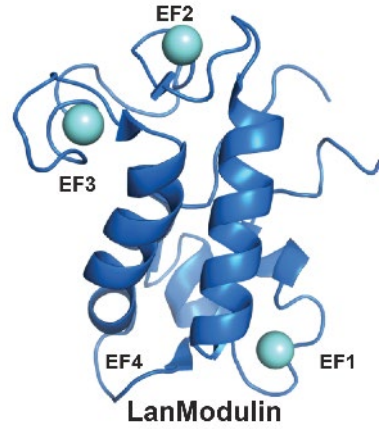
American Elements 2011.

US Imports > 90% REEs from China



Scientific American, 2019.

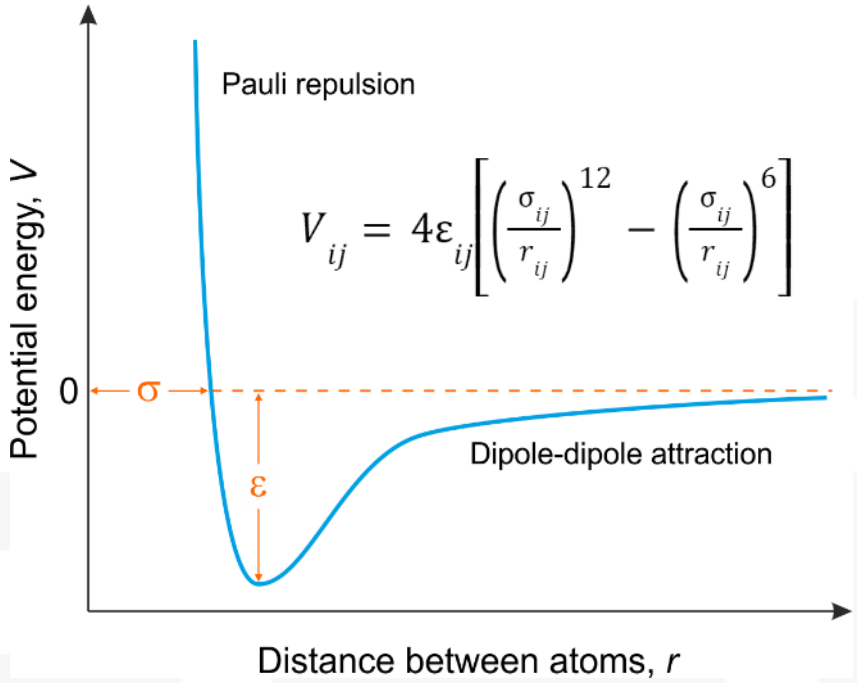
- Traditional REE extraction poses severe environmental impact
- US has virtually no domestic production of REEs today
- US REE supply chain security is at risk
- Protein-based REE extraction method could increase production in the US
- Lanmodulin (LanM) is a natural REE binding protein

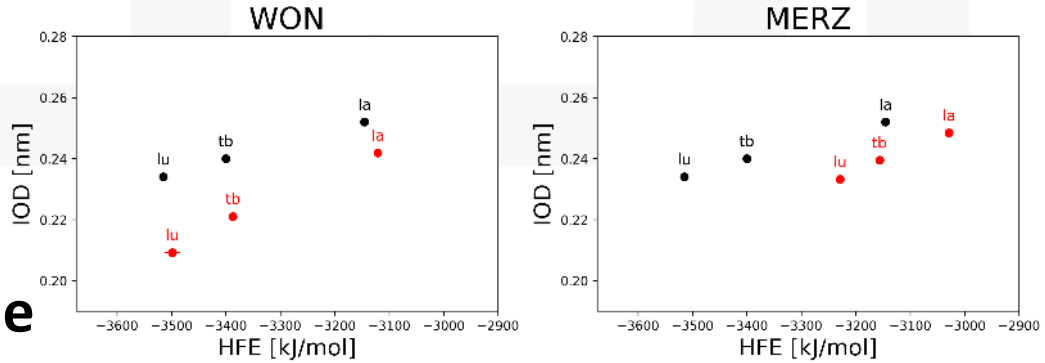


What Even Are Force Fields?

- Function that models the movement/interactions of atoms in a system
- We are interested in **nonbonded**, **Van der Waals** interactions of REE ions themselves
- Two components:
  - $\boldsymbol{\sigma}$: Distance where repulsive and attractive forces cancel out
  - $\boldsymbol{\varepsilon}$: Maximum attraction before repulsive forces kick in
- Accurate force fields create accurate descriptions of ion coordination with peptides/proteins

Force fields need to accurately capture both the coordination energy *and* coordination structure



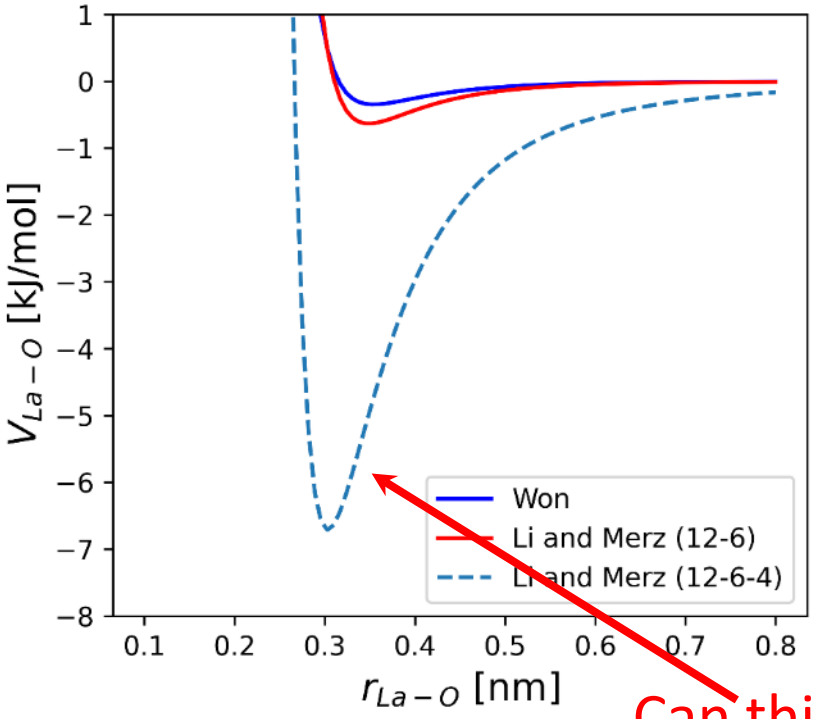


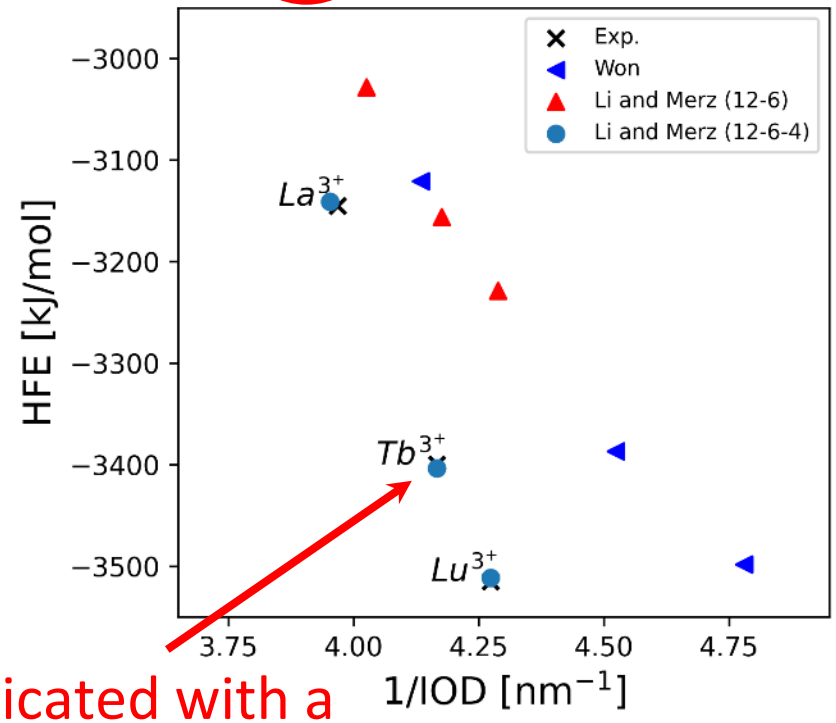
A Temporary Solution

- Li and Merz (2015) found adding a quartic term improves forcefield

$$V_{ij} = 4\epsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right] - \left(\frac{C_{ij}}{r_{ij}}\right)^{4}$$

IMPLEMENTATION IS NON-TRIVIAL!!!





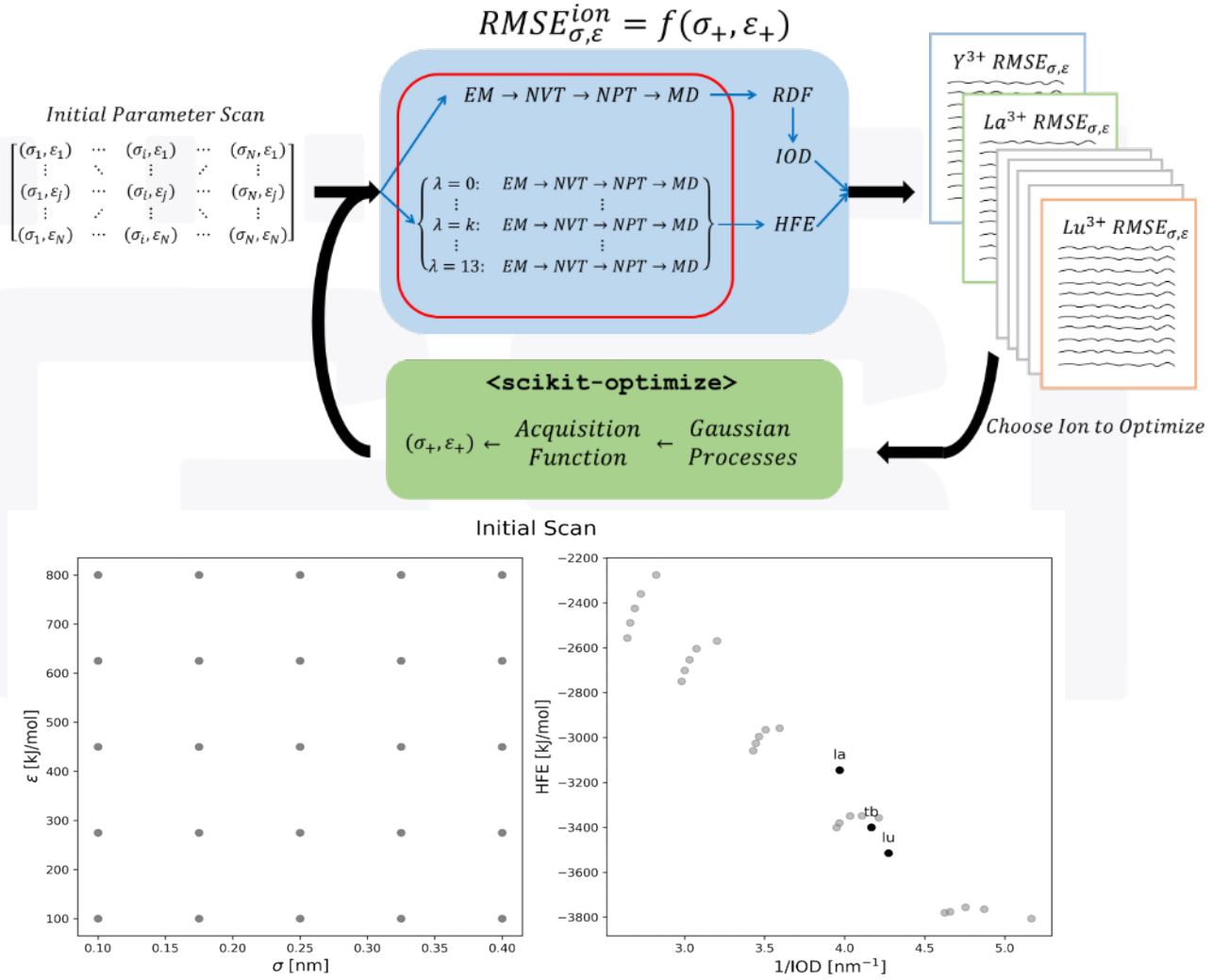
Can this be replicated with a "standard" 12-6 potential?

Bayesian Optimization

- Usually employed to optimize expensive-to-evaluate functions
  - Our “function” is a collection of simulations:
    - *Error = f (σ, ε)*

- Implemented in python package `sk-opt`
- Evaluate function at certain (σ, ε) and give results to the “optimizer”
- It then predicts the next (σ, ε) to evaluate

Can choose to optimize any ion and re-use all previous data

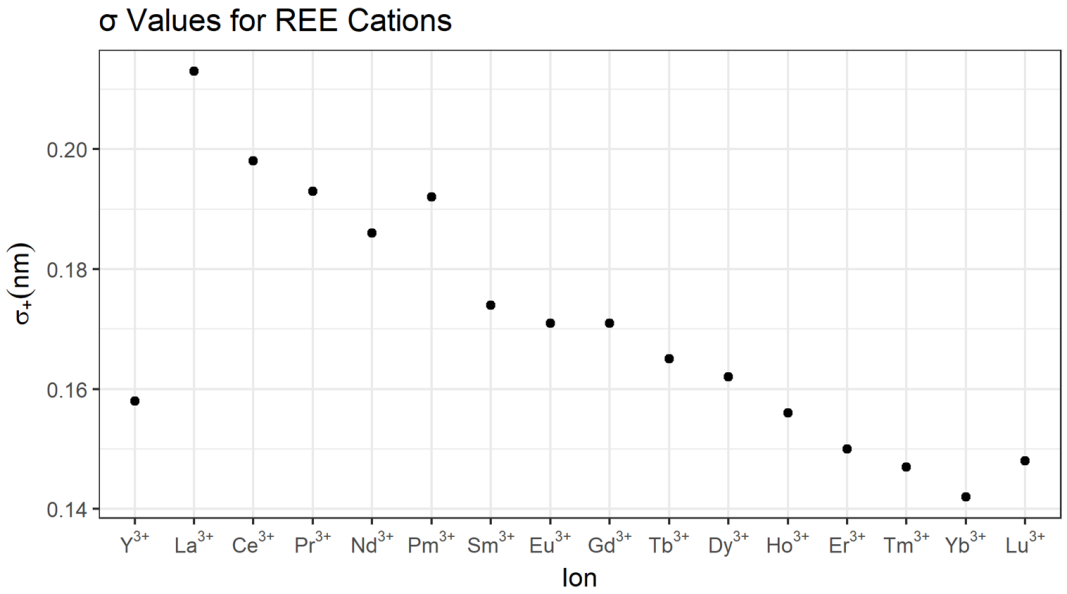


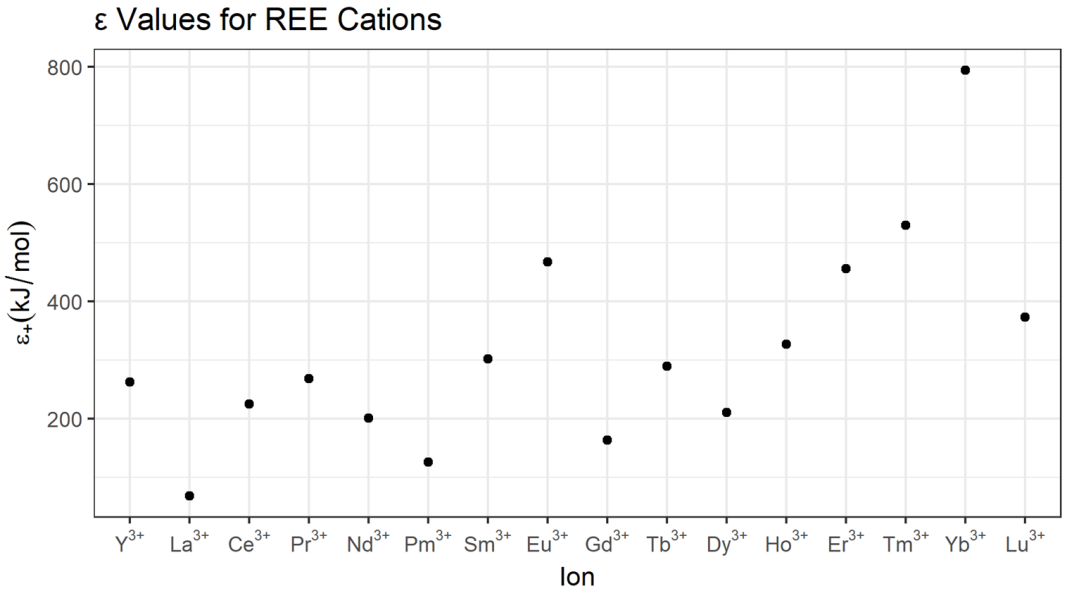
Problem Solved!... Right?

- One catch: Only truly accurate in a system **with only water**
- Cross-interactions with other ions/proteins are much too strong due to high epsilons
- Can't change epsilons because it would change the coordination energy and structure

Solution: Introduce scaling factors into the calculations of these cross-interactions (mixing rules)

Fyat & Netz, "Ionic force field optimization based on single-ion and ion-pair solvation properties: Going beyond standard mixing rules", *J. Chem. Phys.*, 2012

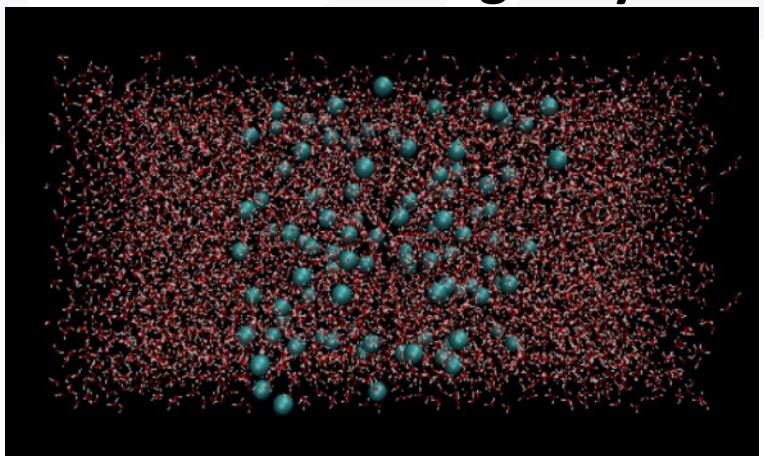




Fixing the Mixing (Rules)

- 2 primary candidates to scale: Chloride anions and protein EF hand loops
- Chloride Anions:
  - Set up invisible walls felt only by the ions and measure the osmotic pressure
  - Calculate the osmotic coefficient and compare to literature values
- Protein:
  - Measure the binding affinity via Free Energy Perturbation (FEP)
  - Compare to literature values

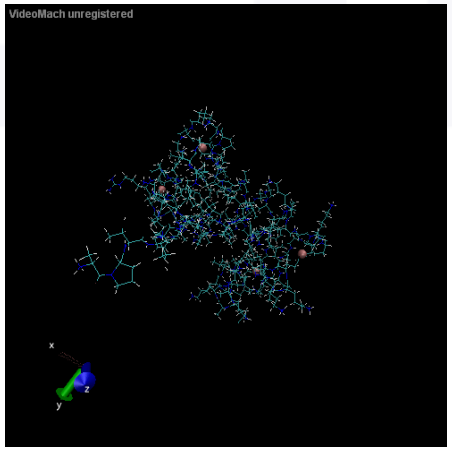
But why guess when we can optimize! We can use the same optimizer to intelligently find the correct scaling factors, similar to before!



$$\sigma_{ij} = \frac{1}{2}(\sigma_{ii} + \sigma_{jj})$$

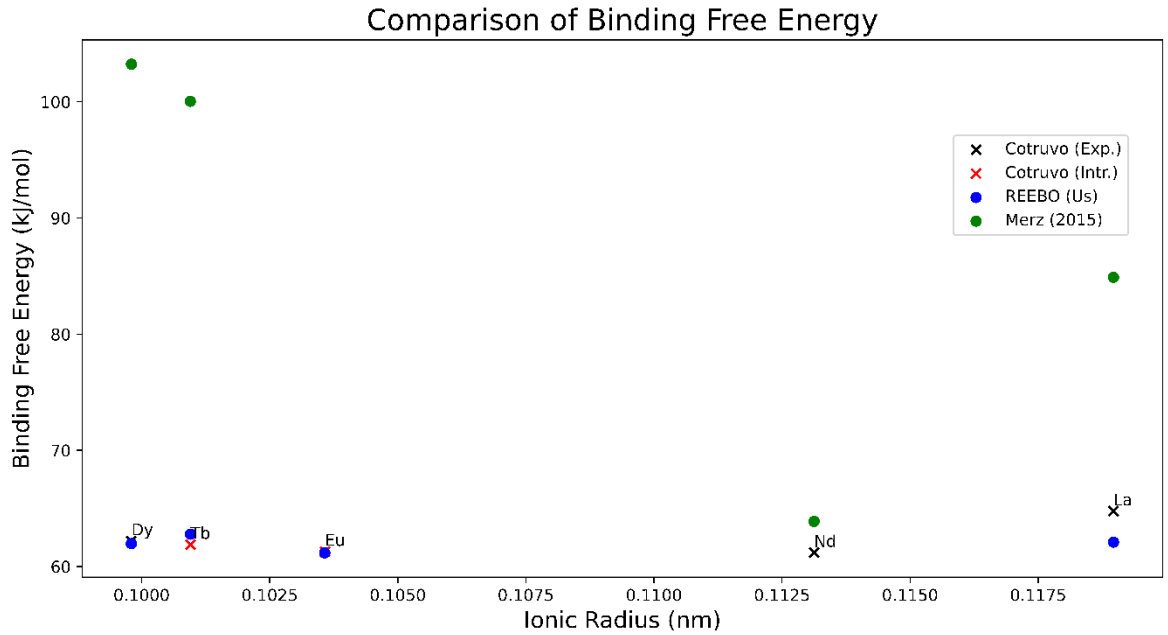
$$\epsilon_{ij} = (\epsilon_{ii}\,\epsilon_{jj})^{1/2}$$

The Lorentz-Berthelot mixing rules. These are **specific** to **two types** of atoms (one will be REE ion)



Conclusions

- Energy values are much more in line with experimental values
  - We can (finally) create working models with REEs
- We can use the same optimizer for a modular workflow
  - Potential uses for other projects



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