



Investigation of Rare Earth Elements Mobility Using Molecular Dynamics

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Changing the World's Energy Future

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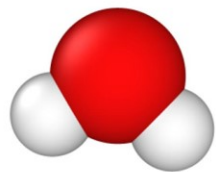
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^{*}Michigan Technological University | (B611) Modeling and Simulation | ¹Idaho National Laboratory, ²University of Wyoming

Motivation and Objective

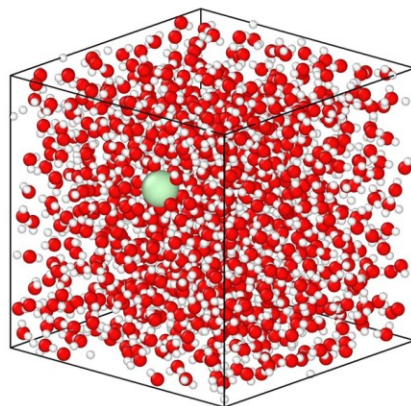
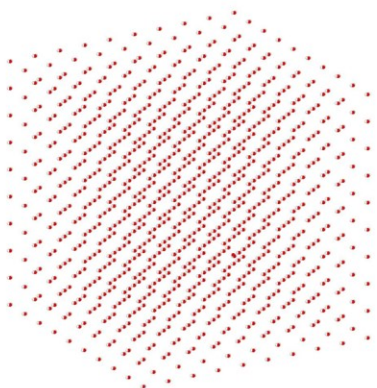
- Rare Earth Elements (REE) are critical many applications (e.g., permanent magnet motors) ^[1]
- Effective separation of REEs is a challenge
- Research on REEs mobility in water-based solvents is necessary to design effective separation processes
- Research objective is to determine the key kinetic and thermodynamic parameters, including diffusion coefficient and hydration shell, under the influence of external electric field.

Molecular Dynamics Framework

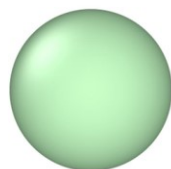


H₂O molecule

Replicate 



 **Densify**



Metal Ion [2]

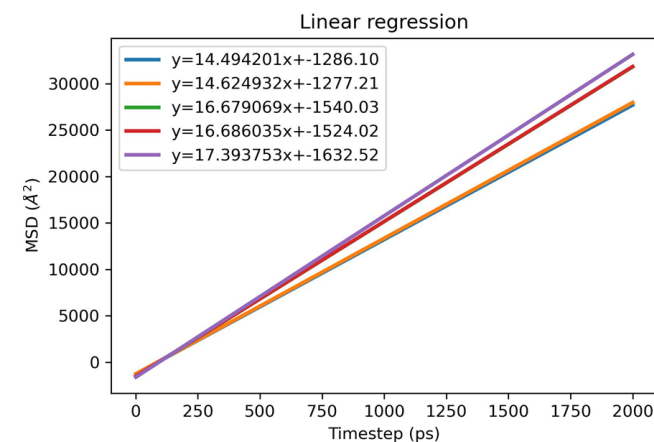
at 298 K, 1 bar

NVT Ensemble

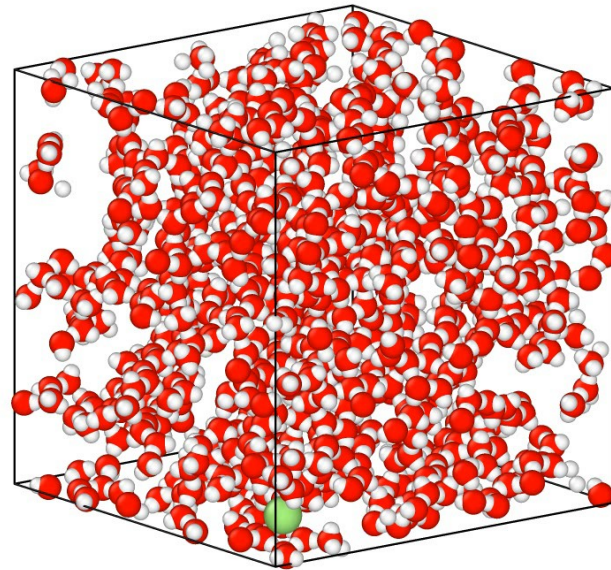
Calculation

- Density
- Mean square displacement
- Coefficient of Diffusion
- Hydration number
- Radius of hydration shell

Analysis 

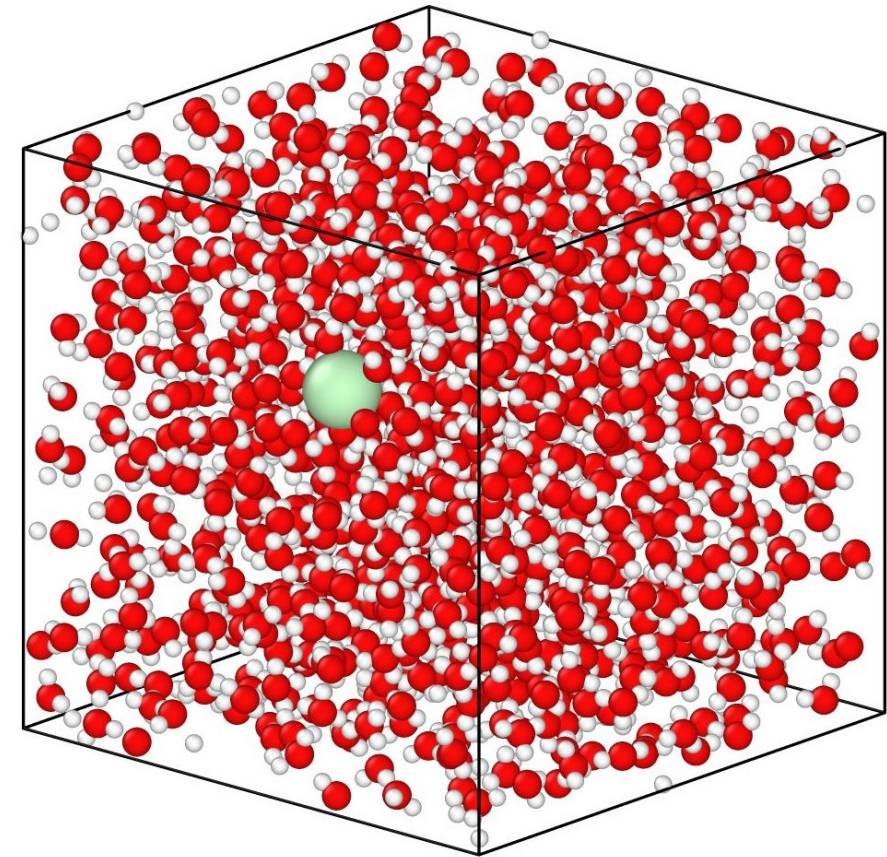


Mixing and Densification

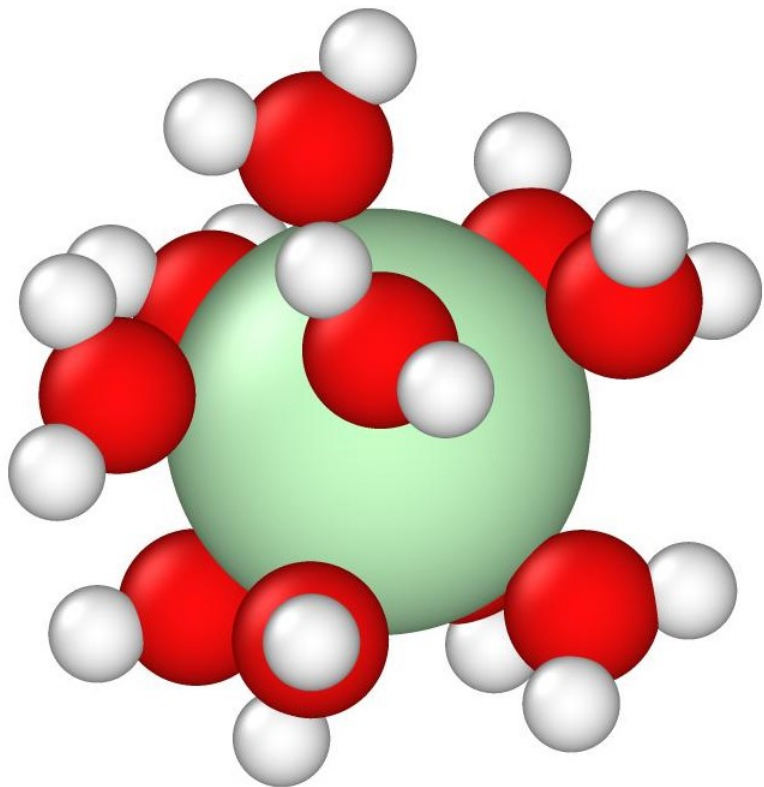


Water – Ln³⁺ model

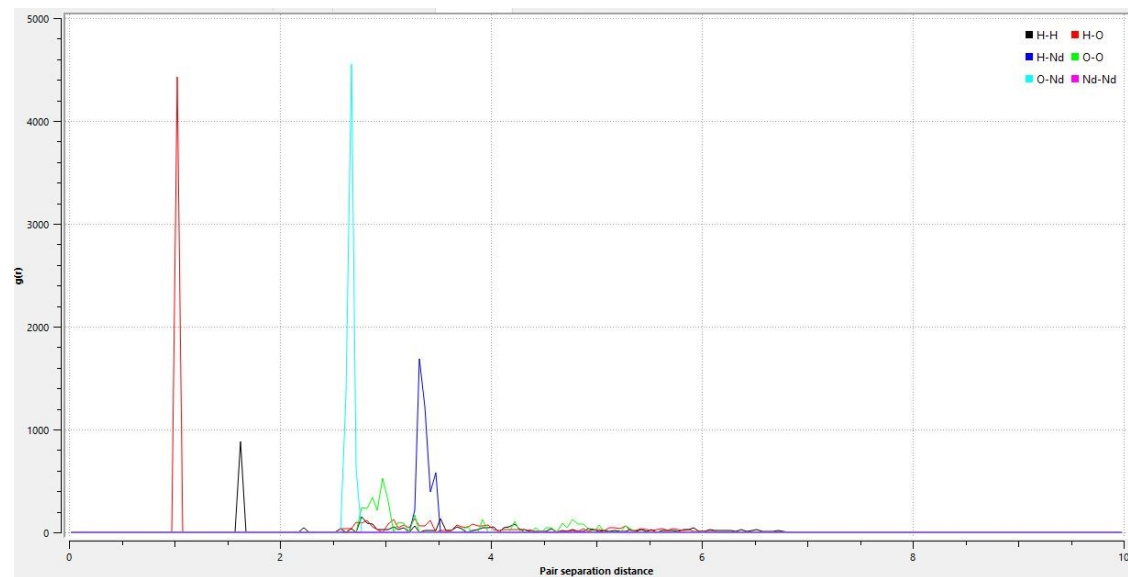
- Number of water molecules: 1000
- Number of Ln³⁺ ions: 1
- Number of atoms: 3001
- Target density: 0.997 g/cc
- Predicted density
 - Water: 1.011 ± 0.002 g/cc
 - Nd³⁺: 1.024 ± 0.003 g/cc
 - Dy³⁺: 1.032 ± 0.003 g/cc



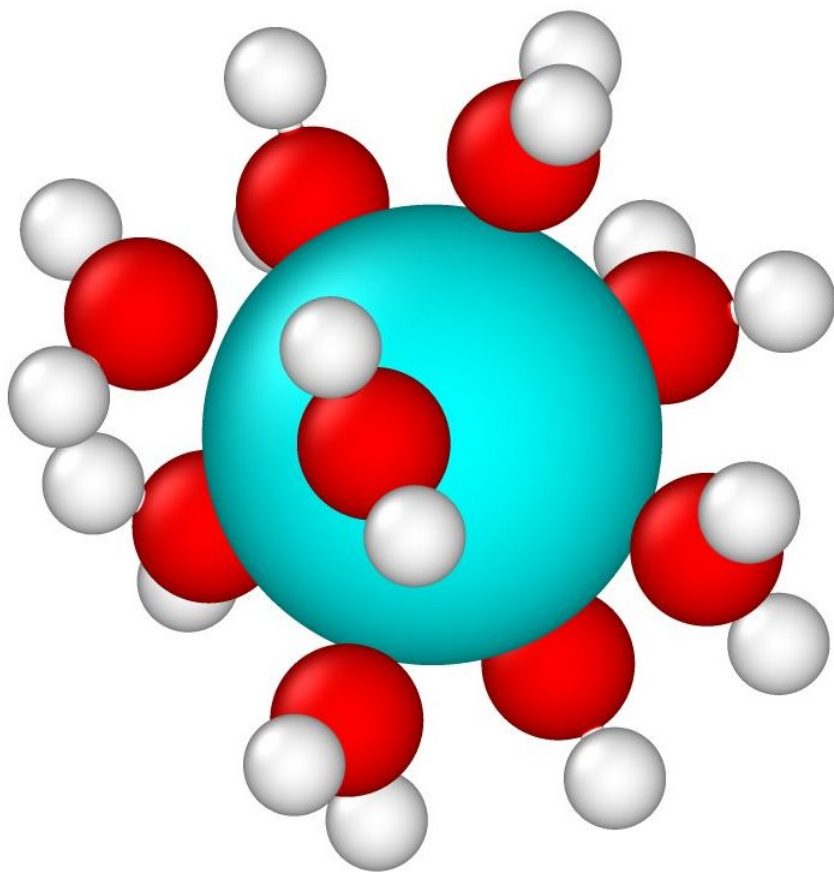
Hydration shell



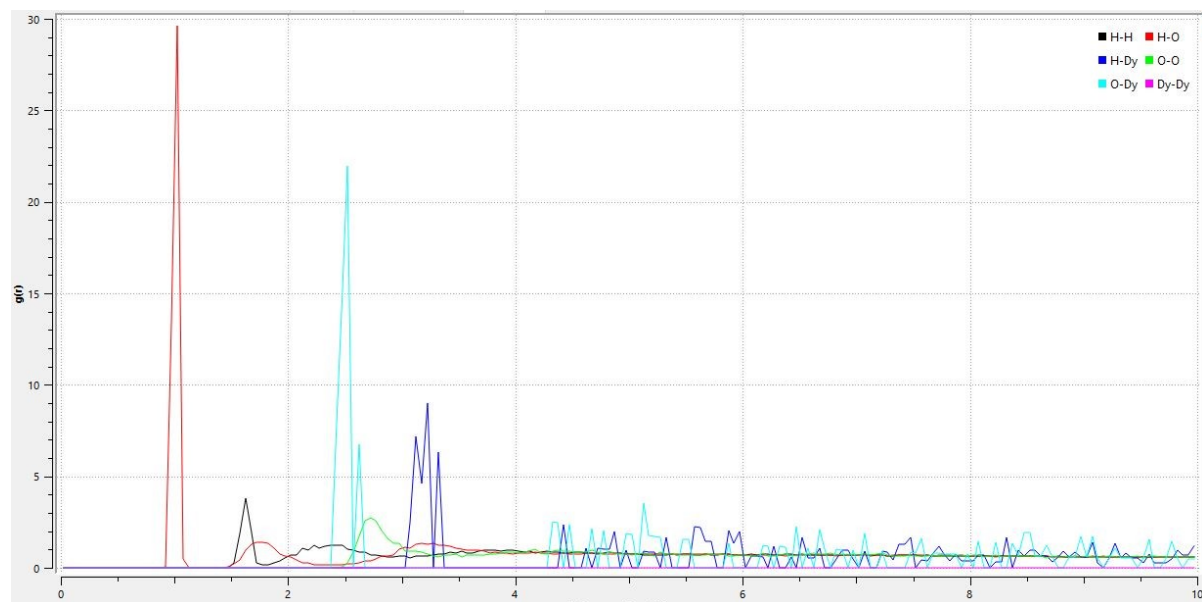
- Number of water molecules: 10
- Radius of 1st hydration shell: 2.69 Å



Hydration shell

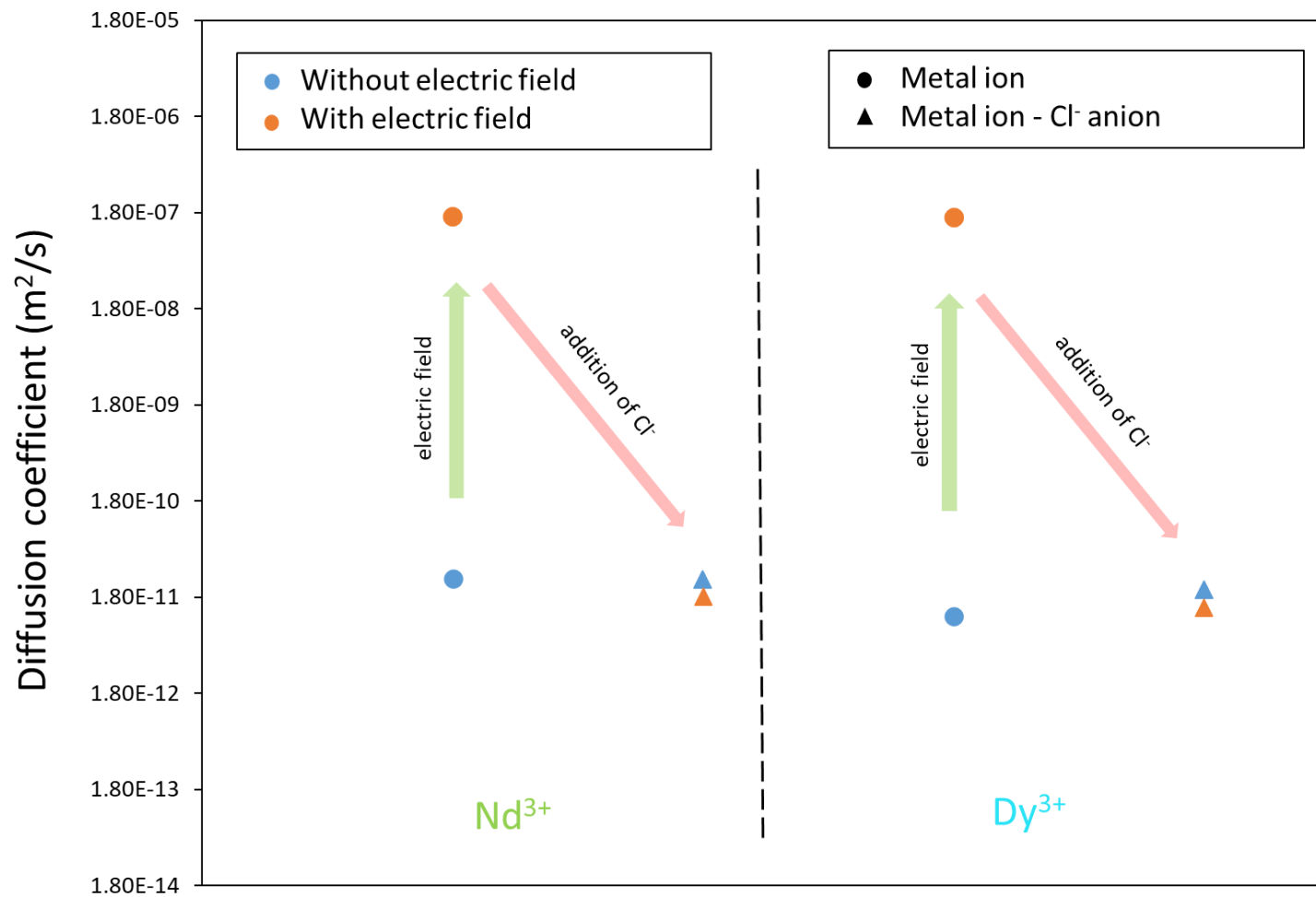


- Number of water molecules: 9
- Radius of 1st hydration shell: 2.48 Å



Diffusion coefficients of metal ions

Comparison of diffusion coefficient



Conclusion

- Diffusion coefficient increases due to electric field in pure water
- Addition of Cl^- anions affects influence of electric field
- Insights on mobility of ions that helps experimentalist to streamline the processes for effective separation of REEs



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