INL/EXP-22-68333-Revision-0

Investigation of Rare Earth Elements Mobility Using Molecular Dynamics

July 2022

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Investigation of Rare Earth Elements Mobility Using Molecular Dynamics

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[*]**Michigan Technological University | (B611) Modeling and Simulation** | [1] Idaho National Laboratory, [2]University of Wyoming

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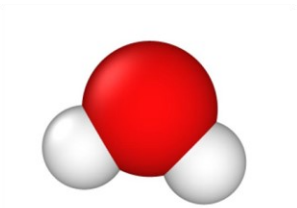
Motivation and Objective

- 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.

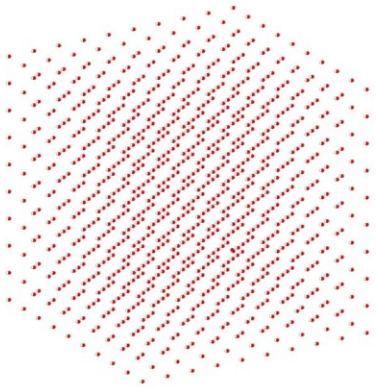
[1] Z. Chen et al., J. Environ. Chem. Eng., 10 (2022) 107104

Molecular Dynamics Framework

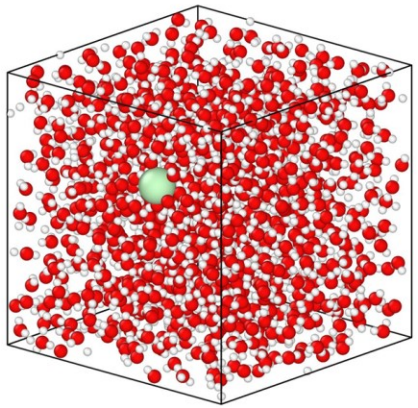


H_2O molecule

Replicate



Densify



Metal Ion [2]

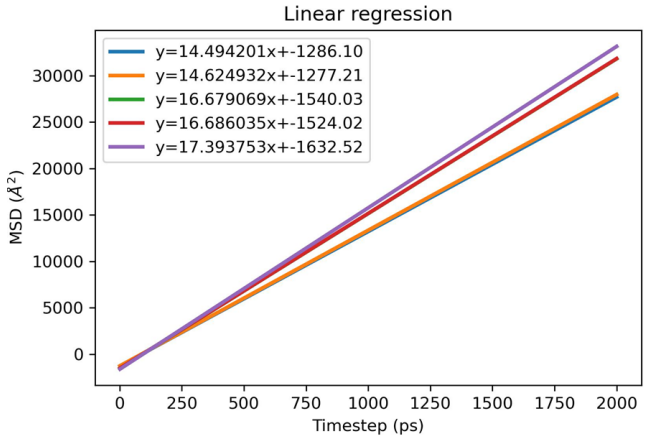
at 298 K, 1 bar

NVT Ensemble

Calculation

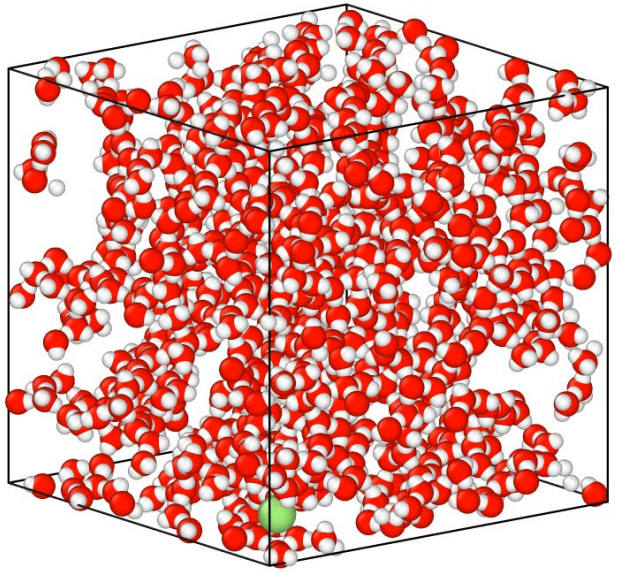
- Density
- Mean square displacement
- Coefficient of Diffusion
- Hydration number
- Radius of hydration shell

Analysis



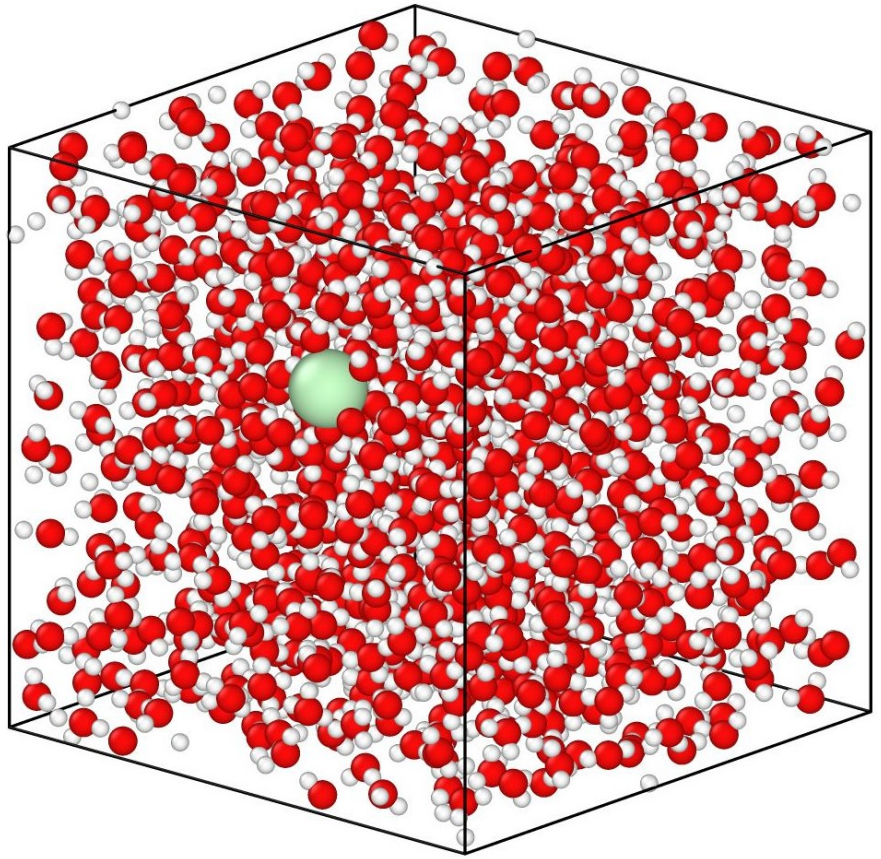
[2] V. Migliorati et. al., Inorg. Chem. 2017, 56, 6214−6224

Mixing and Densification

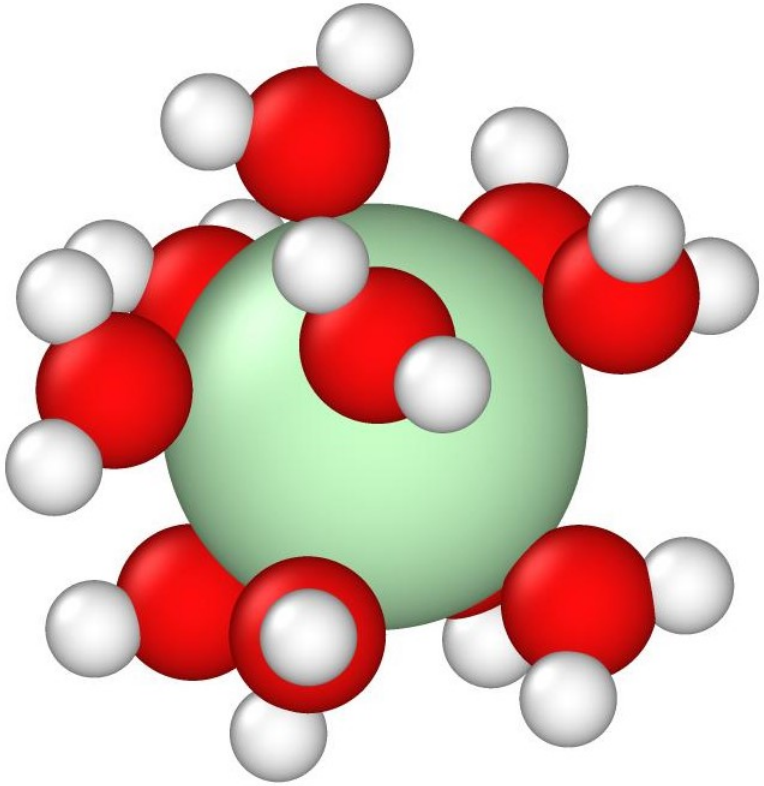


Water – Ln^{3+} model

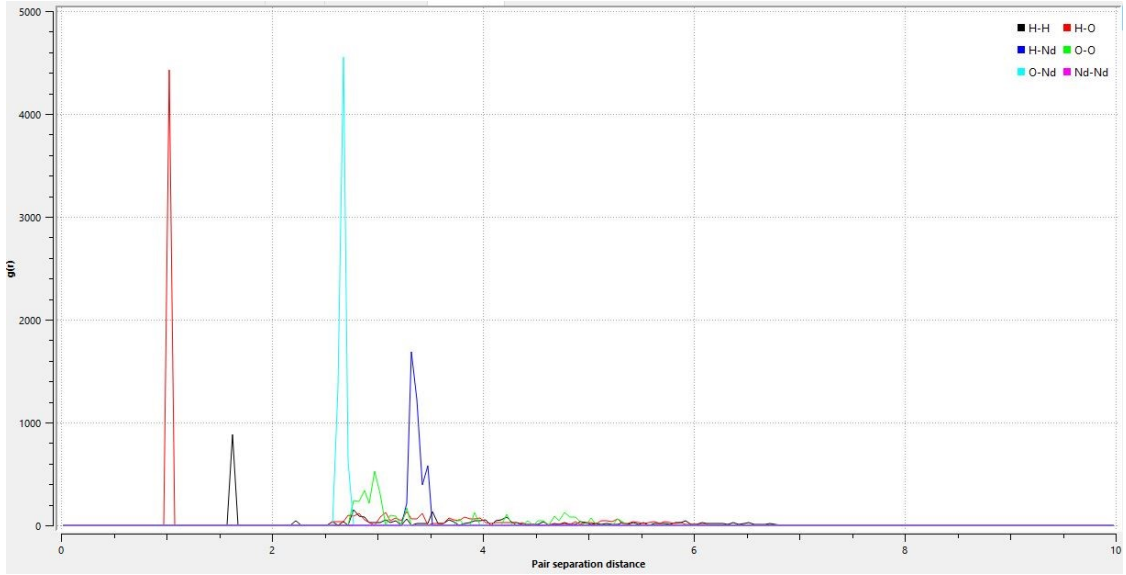
- Number of water molecules: 1000
- Number of Ln^{3+} ions: 1
- Number of atoms: 3001
- Target density: 0.997 g/cc
- Predicted density
  - Water: 1.011 ± 0.002 g/cc
  - Nd^{3+}: 1.024 ± 0.003 g/cc
  - Dy^{3+}: 1.032 ± 0.003 g/cc



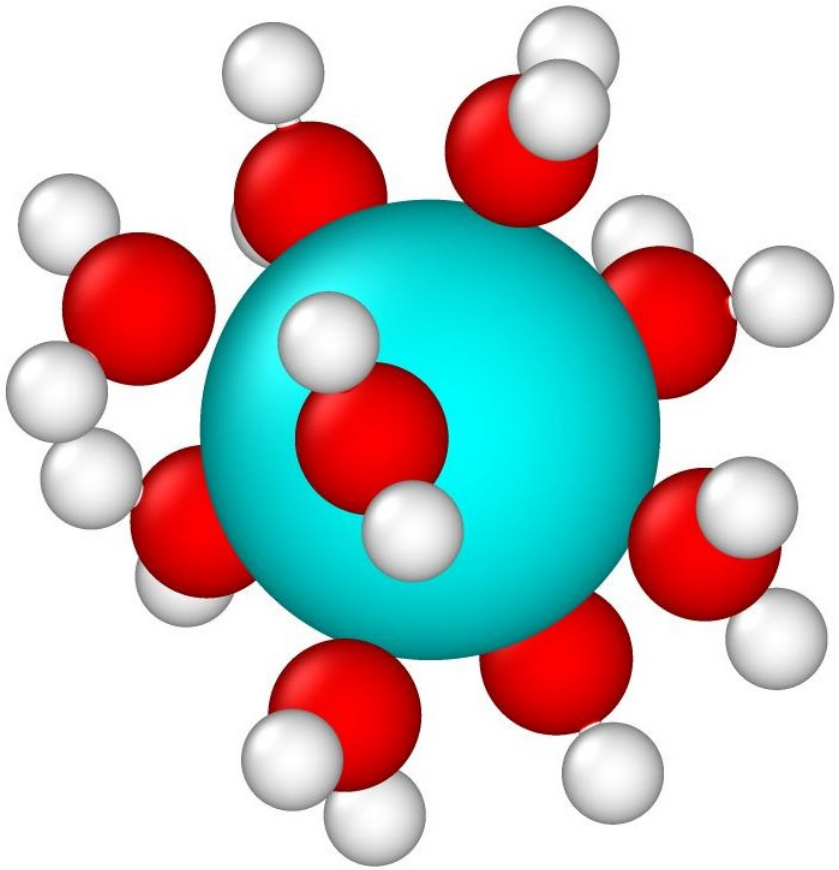
Hydration shell



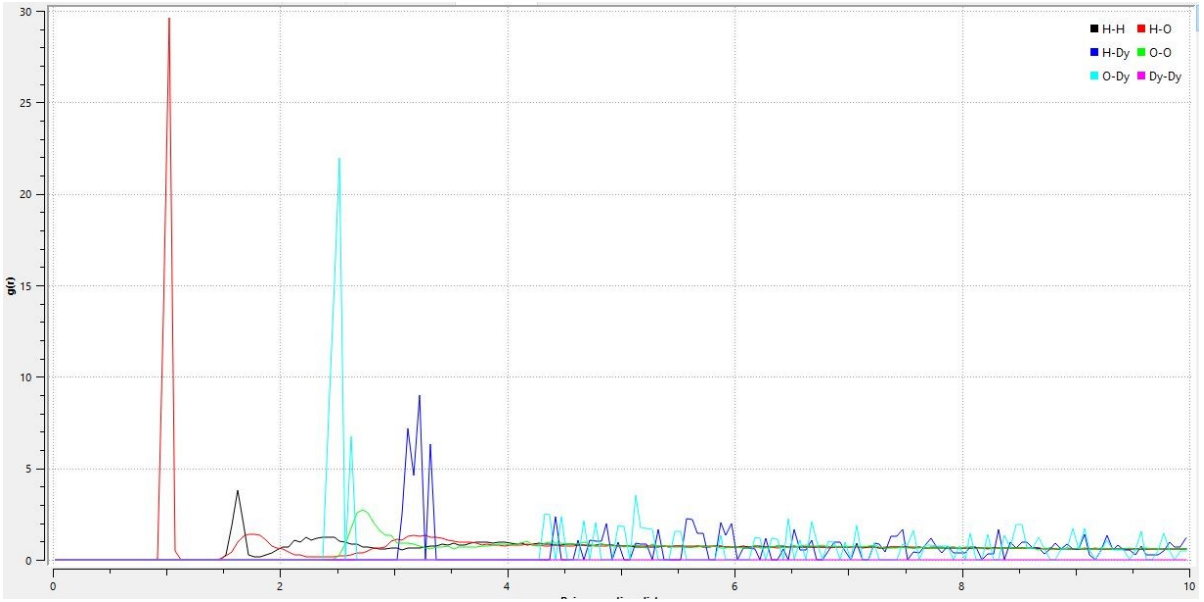
- Number of water molecules: 10
- Radius of 1st hydration shell: 2.69 Å



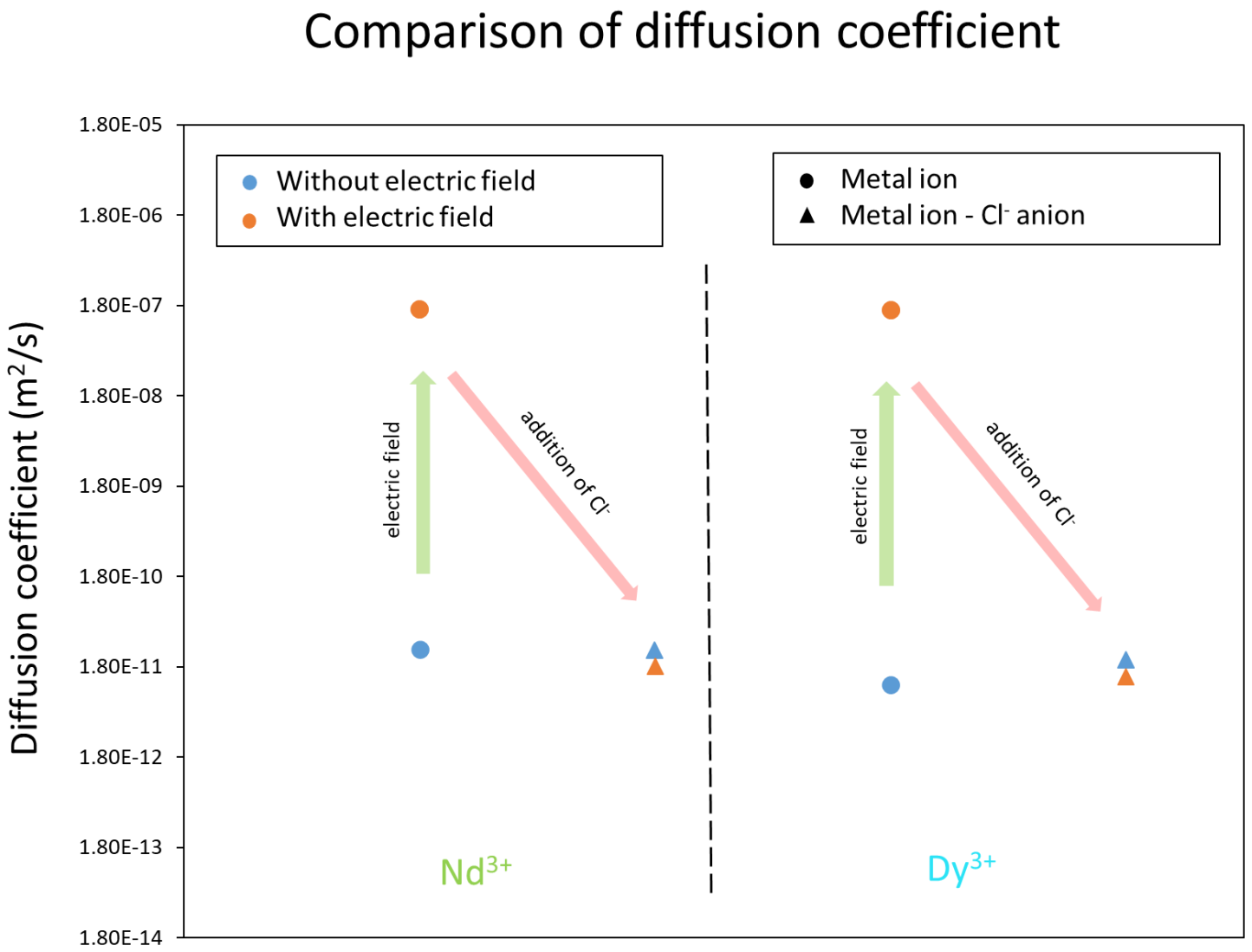
Hydration shell



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



Diffusion coefficients of metal ions



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

Acknowledgements

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