INL/EXP-22-68258-Revision-0

Investigation of Rare Earth Elements Mobility Using Molecular Dynamics

August 2022

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Idaho National Laboratory

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Investigation of Rare Earth Elements Mobility Using Molecular Dynamics

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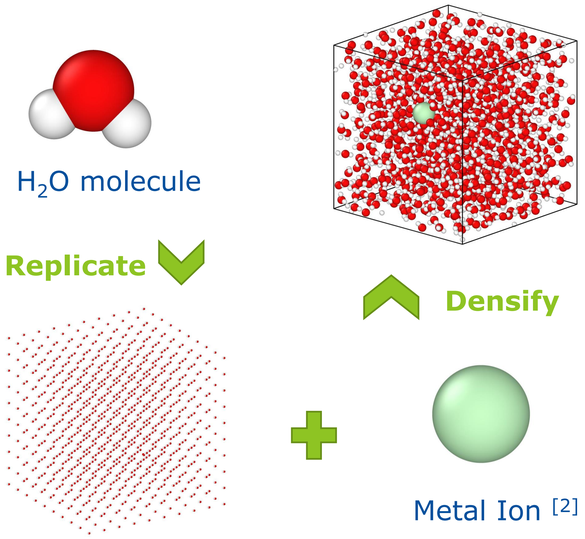
Significance/Objective

- 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



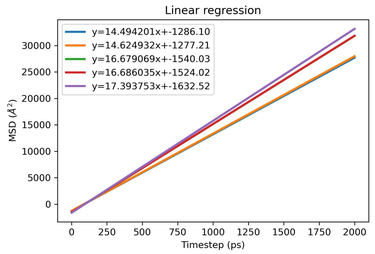
at 298 K, 1 bar

NVT Ensemble

Calculation

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

Analysis

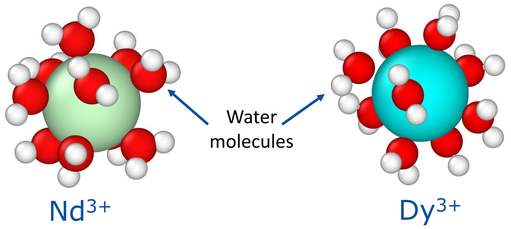


Python Scripting

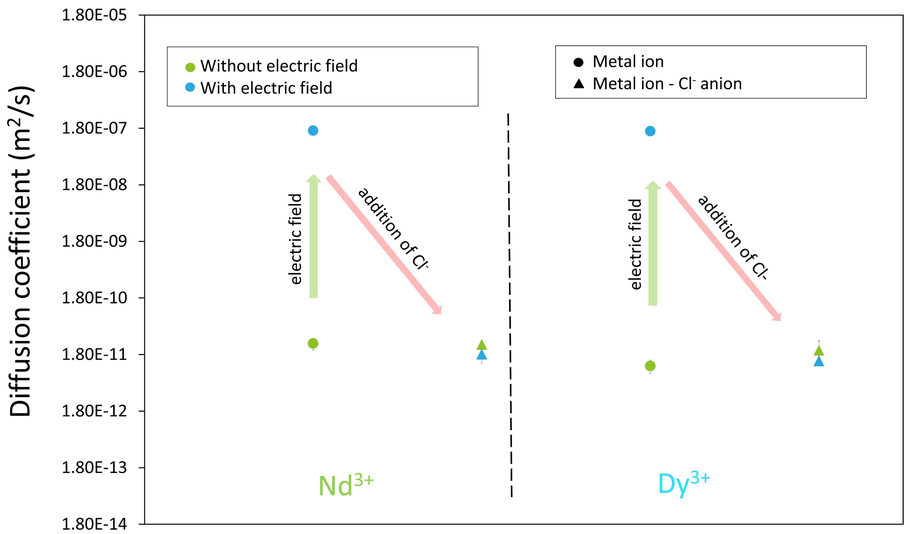
Results

Ion	Nd^{3+}	Dy^{3+}
Density (g/cc)	1.028	1.032
Number of water molecules	10	9
Radius of hydration shell (Å)	2.69	2.48

Hydration shell of Nd^{3+} and Dy^{3+} ions



Diffusion coefficients of Nd^{3+} and Dy^{3+}



Conclusion

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

Acknowledgements

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