

# **Activity Coefficients from Vapor-Liquid Interfaces: A Molecular Dynamics Approach for Separation Chemistry**

solution

Extractant

aggregates

in the

organic



lons and

solution

molecules in

Aggregates

Mesoscopic

**properties** 

# Context

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Understanding **solvent extraction** – Recycling of rare earth elements and spent nuclear fuels









A multiscale approach provides mesoscopic thermodynamic properties

**1** A

10 Å

10<sup>2</sup> Å





 $(NO_3)_3(H_2O)_mL_m$ 

 $C_{\rm Dy^{3+}} C_{\rm NO_2^{-}} {}^3 x_{\rm H_2O} {}^m$ 

**Concentrations** 

DMDOHEMA



### **Methods and concepts**



## Aqueous dysprosium nitrate $Dy(NO_3)_3$ solutions <sup>(2)</sup>



#### **Organic phases – Binary Mixtures of DMDOHEMA and** *n***-heptane**

Molecular dynamics simulation of liquid-vapor equilibria of organic solvent phases containing:









**Outlook and conclusion** 

#### Aggregation of DMDOHEMA in the organic phase relies on the availability of water<sup>(3)</sup>

Increasing

cost

computational

- Solvent activities in binary mixtures of *n*-heptane and DMDOHEMA show ideal behavior and follow Raoult's law in good agreement up to a high extractant concentration
- Attractive and repulsive interactions in the mixtures cancel out

#### • Aqueous salt solutions: Results from molecular dynamics simulation are in good agreement with experimental data for different nitrate salts. This approach can be used for the validation of force fields for MD simulation with respect to thermodynamic properties.

- Organic Phases: Method has been successfully applied on binary mixtures (n-heptane) and DMDOHEMA, but also ethanol and water<sup>(4)</sup>). Allows accessing more complex organic solvent phases containing water and ionic species.
- > Simulation of activity coefficients of complex solutions with volatile solvents for understanding solvent extraction

# References

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