

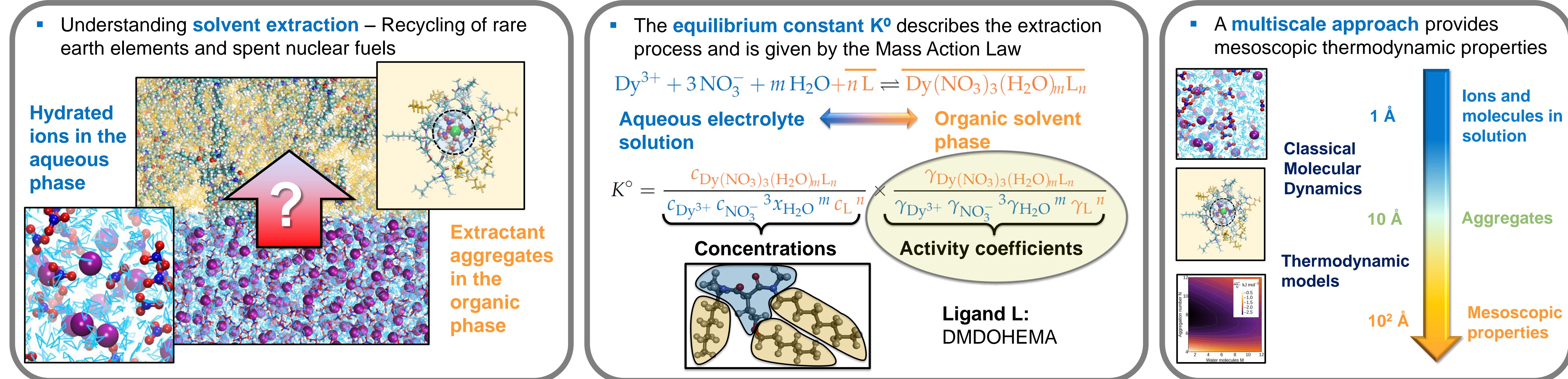
Activity Coefficients from Vapor-Liquid Interfaces: A Molecular Dynamics Approach for Separation Chemistry

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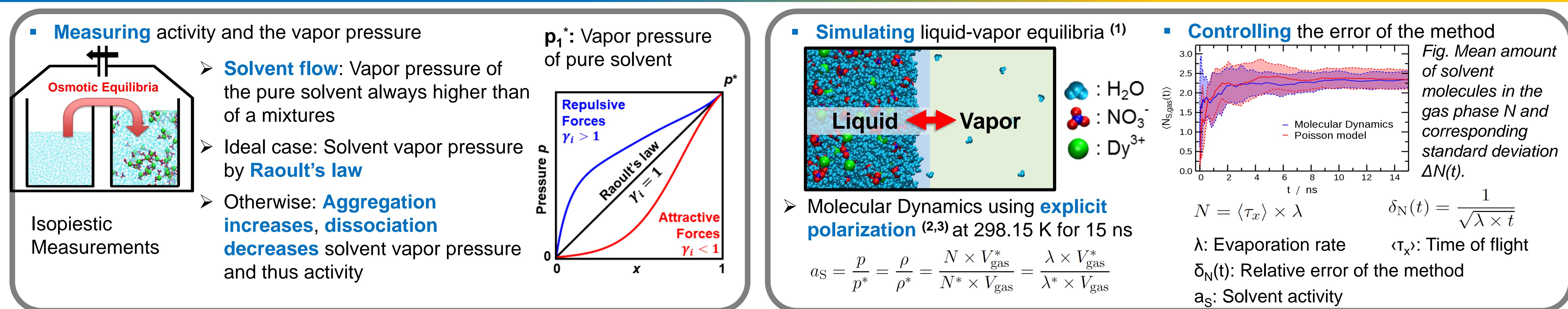
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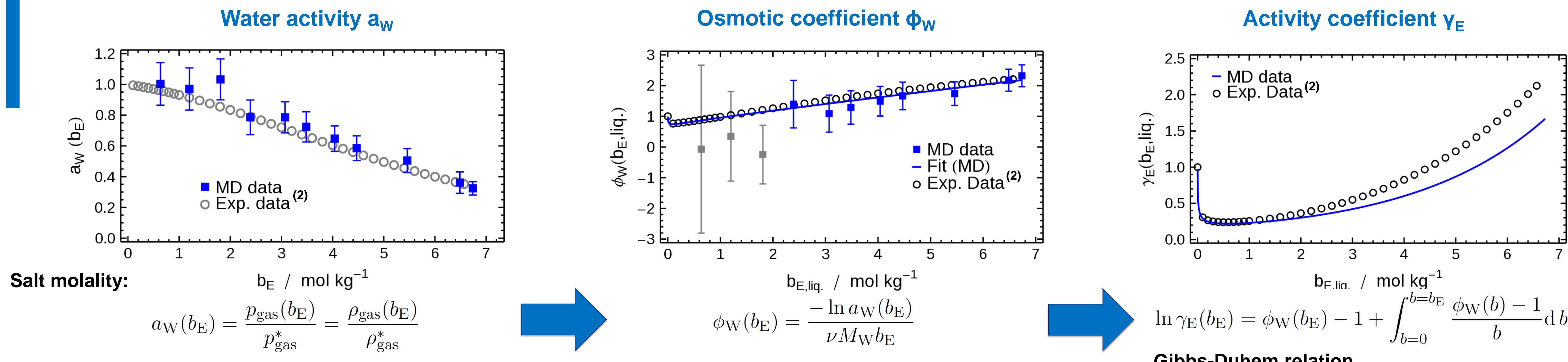
Context



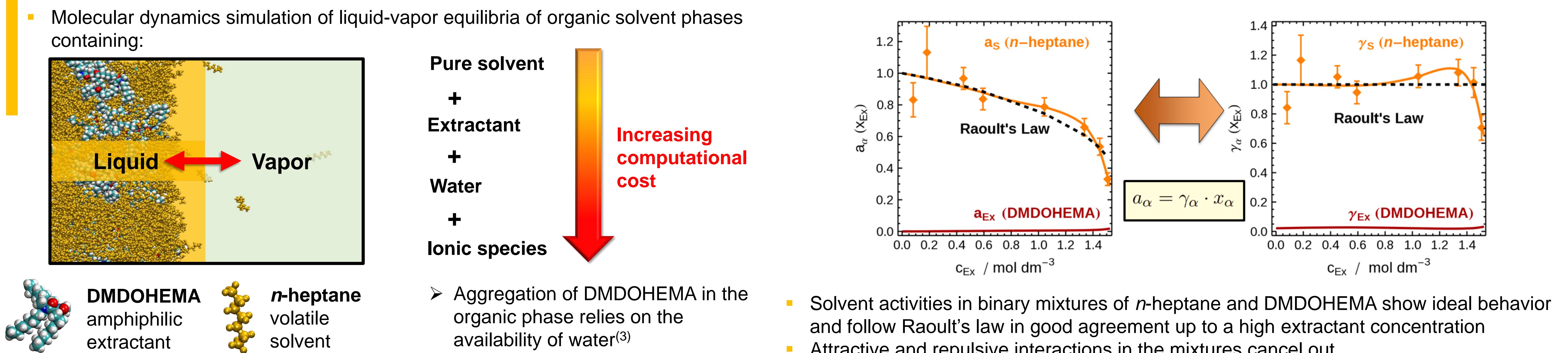
Methods and concepts



Aqueous dysprosium nitrate $Dy(NO_3)_3$ solutions⁽²⁾



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



Outlook and conclusion

- 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⁽⁴⁾). 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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