# OLI Software: Thermodynamic Modeling Tool for Critical Materials

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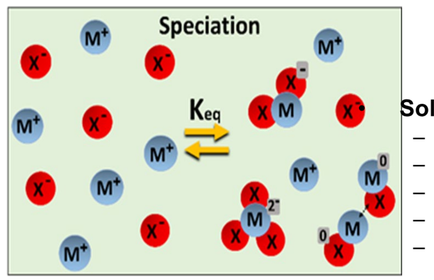
## Background

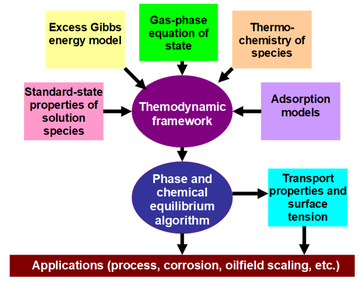
- **Application of Rare Earth Elements (REE) in high tech, defense, and clean energy technologies has provided an overwhelming impetus for scientific studies over the last few decades**
  - Unique magnetic, luminescent, electrical, and catalytic properties of the elements
- **Direct impact in clean energy technologies like electric vehicles (EV) and wind turbines**
  - e. g., 93% of 2 million EVs sold in 2018 utilize permanent magnet traction motors; estimates indicate that there could be ~150 million EVs on road by 2030
- **Supply for primary mineral sources is subject to geopolitical constraints**
  - Increasing interest in diversifying the supply, recycling and substituting critical REEs
- **Thermodynamic modeling of aqueous solution chemistry and phase equilibria are essential for aiding the development of novel processing technologies**
  - Extractive metallurgy, technospheric mining, recycling, and separations

## Theory and Model

- **Mixed-Solvent Electrolyte (MSE) theoretical framework was developed by combining standard-state properties of all species and an excess Gibbs energy model for solution non-ideality**
  - The model parameters are obtained from experimental SLE (solubility), VLE (osmotic coefficient) and caloric (solution heat capacity) data

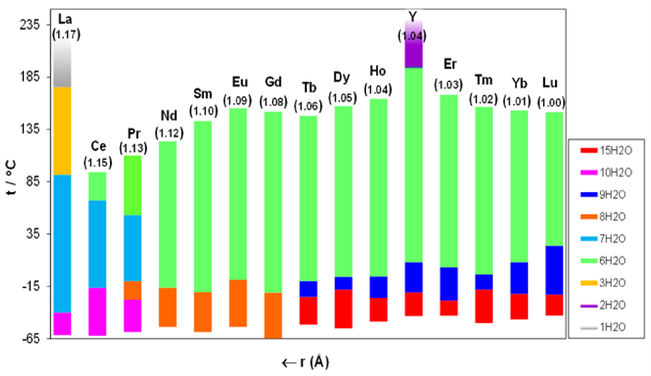



**Solution chemistry equilibria**
- Acid-base
- Complexation
- Redox
- Solid phase precipitation
- Surface complexation and other adsorption phenomena

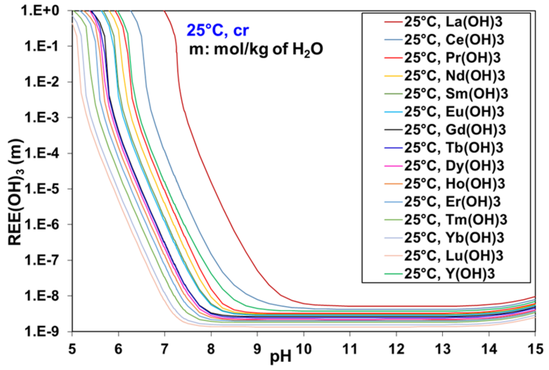



- **Modeling of fundamental phase behavior and thermodynamic properties of REE containing systems using MSE model**

**Stability regions of hydrated REE chlorides**



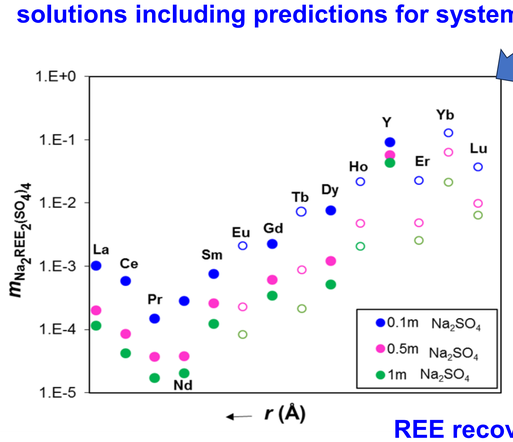

**Solubilities of crystalline REE hydroxides**

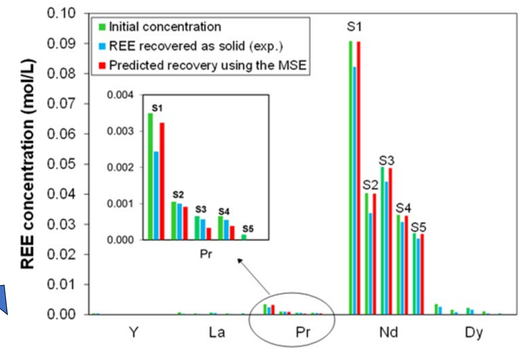



## Results

- **Recovery of REE from hard disk drives using a reusable extraction medium**

**Solubilities of double salts as a function of crystal cationic radii in $Na_2SO_4$ solutions including predictions for systems for which data are not available**

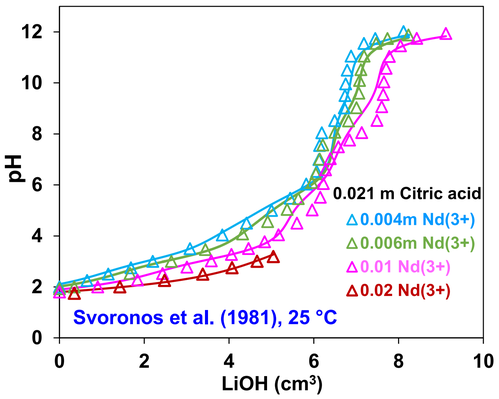


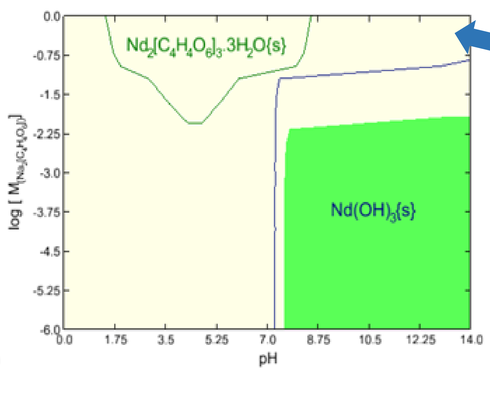

**REE recovery by precipitation as double sulfate salts after leaching using HCl to recycle REEs from shredded hard disk drives**

- **Organic ligand driven recovery of REE through dissolution and precipitation**

**Titration curves for $Nd^{3+}$ containing system in the presence of citrate ligand**



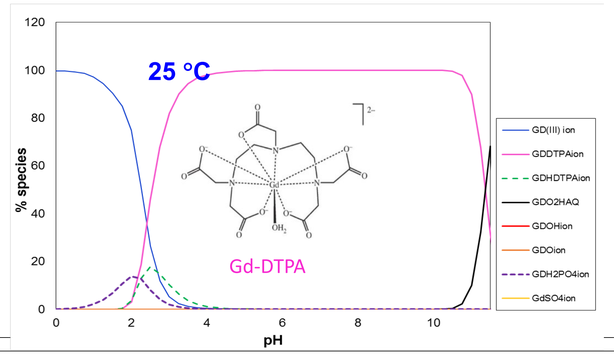

**Stability diagram predicting the solubilization window for REE from its precursors**



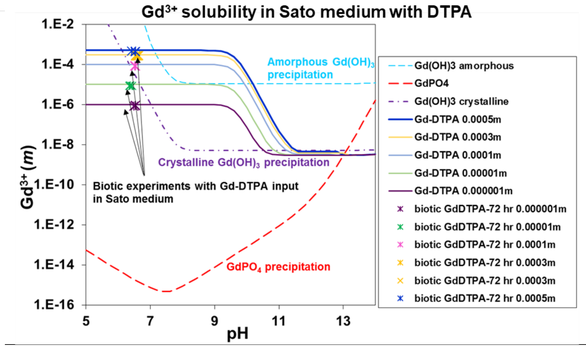

**"Sweet spot" where Nd is complexed and dissolved**

- **Study on environmental impacts of REE processing**

**Gd complexation with DTPA**




**Prediction for solubility of Gd in biological medium**




## Conclusion

- **MSE model within OLI Software provides thermodynamic models for a large number of REE compounds which allows novel process development**