**Motivation**

- Thermal limitations on capabilities, efficiencies, and power densities have been identified as a DoD Power and Energy Gap. If successful, this project will advance a technology (thermal energy storage) with the potential to shrink this gap.
- Heat storage can be used to regulate temperatures of ground vehicle systems (e.g., engine, transmission, electronics).
- Salt hydrates show promise for thermal energy storage (TES).

**Research Questions**

- Which materials have the highest capacities for TES under operating conditions relevant for ground vehicles?
- Can optimal TES materials be efficiently identified by revealing elementary features that control capacity, rates, and stability?

**Objectives**

- Screen thousands of hypothetical salt hydrates for their TES capacities and stability.
- Develop machine learning models for predicting the TES capacity.
- Identify features that strongly correlate with TES performance.

**Approach: High Throughput Screening**

- Generate 5,292 hypothetical hydrates from known crystal structures using cation and anion substitution.
- Calculate enthalpy of dehydration and stability using Density Functional Theory (DFT) calculations.
- Identify promising reactions with high energy density, stability, and low temperature hysteresis.

**Hypothetical Hydrate Generation**

<table>
<thead>
<tr>
<th>Salt Hydrate</th>
<th>MX_{nH2O}</th>
</tr>
</thead>
<tbody>
<tr>
<td>Crystal Structures</td>
<td>MX_{nH2O}</td>
</tr>
<tr>
<td>Cations</td>
<td>MX_{nH2O}</td>
</tr>
<tr>
<td>Anions</td>
<td>MX_{nH2O}</td>
</tr>
<tr>
<td>Hypothetical Hydrates Generated</td>
<td>MX_{nH2O}</td>
</tr>
</tbody>
</table>

**Screening Process**

1. Hypothetical Hydrate Generation
2. DFT Calculations
3. Check Hydrate Structure
4. Assess Stability via Convex Hull
5. Calculate VED, GED, T_Live
6. Hydration Reactions
7. Promising TES Reactions

**Results**

- 3,647 hypothetical hydration reactions characterized.
- 15 promising reactions identified → Invention disclosure filed.

**Performance of Hypothetical Hydrates**

**Interpretable Machine Learning**

- TES performance depends on the enthalpy of dehydration (ΔH).
- Machine learning (ML) performed on hydrate database to predict ΔH.
- 20 feature sets used, some of which contain informative features (i.e., interpretable, generalizable).
  - Informative features: ionic radius, coordination number, etc.
  - Non-informative features: crystal graph representation, identity of cation, etc.

**Future Work**

- Expand study to 786,236 hypothetical mixed-metal salt hydrates.
- Use predictive ML model and active learning to screen with minimal DFT calculations.
- Examine porous materials: opportunity for enhanced power density.
- Collaboration with Eindhoven University of Technology to experimentally verify predictions.