Group 1: Research for Materials Design

Group members:

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Focus (phase-based property data needed to build Composition, temperature, pressure dependent CALPHAD-base databases)

G. B. Olson, 2013
What data and tools are needed for research for materials design?

**Data Needs**
- **CALPHAD Proto Data**
  - Thermodynamic quantities, diffusion mobilities, molar volumes etc.
- **Access to CALPHAD descriptions**
- **Access to Design specifications (Granta -design selection)**
  - Key characterization parameters are missing (e.g. defect information)
- **Property/Performance data (phase-based)**
- **Characterization of synthesis process and quality of material (beyond fundamental properties, TEM characterization, defect characterization)**
- **Better characterization processing**

**Tools**
- **Integrated CALPHAD-type tools with mechanistic tools to predict property and performance**
- **Uncertainty analysis and propagation / Quality of data**
- **Translators**
- **Capture Code/Data - DOCKER instances**

**Physical sample warehouse??**
Key points of Group 1 discussion

• Need to make data curation part of the research workflow

• Access to data can be controlled at different levels during the research project

• Need for basic schemas for materials that the community can build on
  – Processing
  – Characterization
  – Property measurements
Group 1
proposed low barrier activity

• Improved the understanding of raw data formats

• Encourage publication of both CALPHAD TDB (functions) and POP (assessed experimental and computational)

• Agree on common exchange standard data - translators for sharing

• Develop successful cases of data curation
High Barrier Activity

• Materials Lab notebook
Requirements/needs/collaborations to accomplish activity

- Community building activity for DFT data needs (what needs to be save, eg wave functions)
- Community building for data schemas
- Encourage instrument vendors to make data schemas open