Group 1: Research for Materials Design

Group members:

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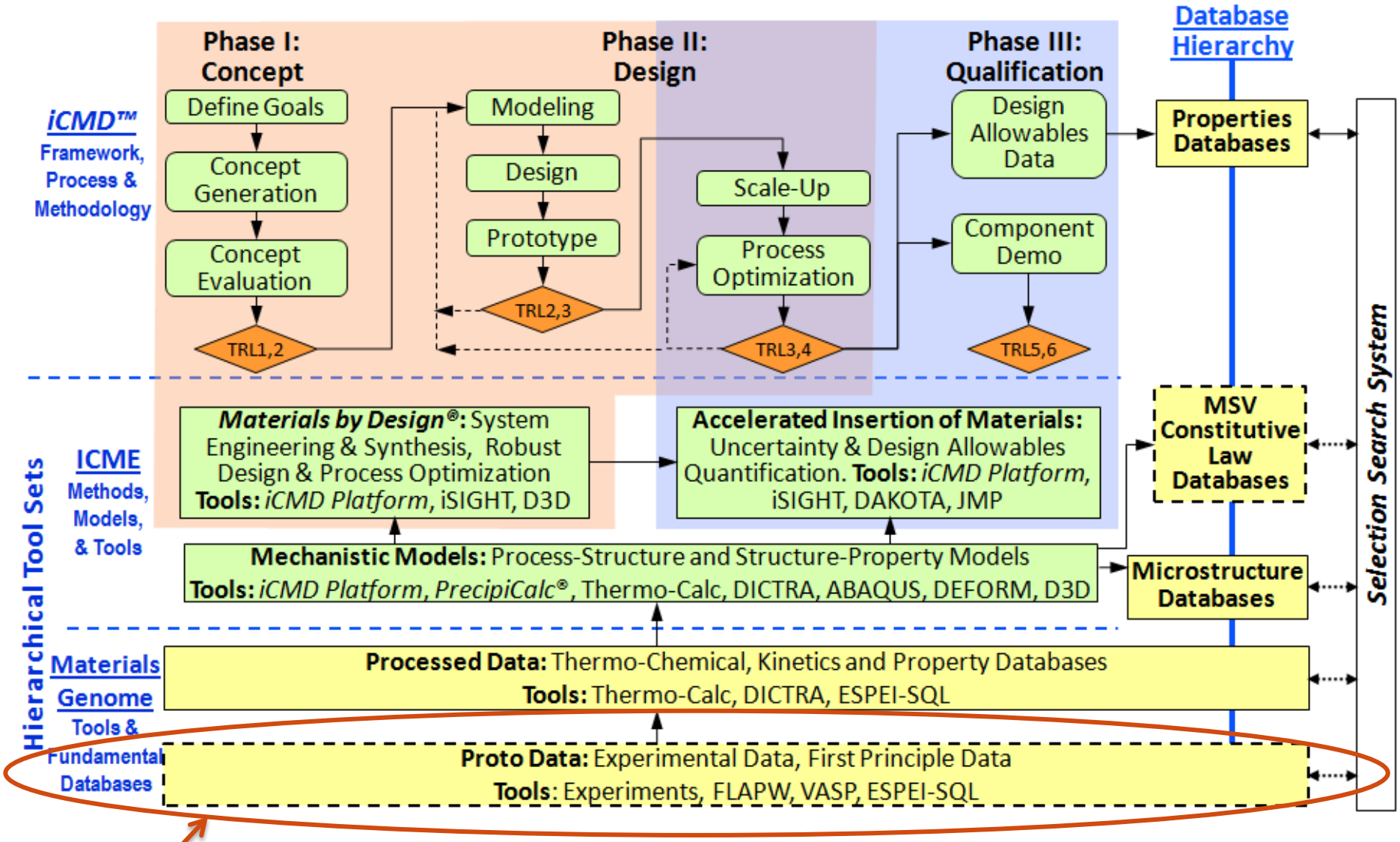

Focus (phase-based property data needed to build
Composition, temperature, pressure dependent CALPHAD-base databases

G. B. Olson, 2013

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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 control 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