Working Group #5: DFT

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Significance of WG's Focus

- DFT integral part of MGI activities
  - DFT data provides connection to many other working groups (e.g., CALPHAD, Materials informatics, polymer?, etc.)
- DFT provides key materials information
- At base of much experimental/computational work – Important to:
  - Find relevant data
  - Interpret data
  - Quantify uncertainty

Summary of WG's Goals

- Many currently existing DFT Databases. We wish to:
- Coordinate Efforts / New Collaborations
- Amplify Impact
- Integrating vs. cross-linking Databases?
- New Databases
  - Example: Effects of vdW functionals (2D materials, polymers)

Technical Requirements/Needs

- "Tons" of CPU time (not necessarily massively parallel machine – need thousands of independent jobs)
  - For example, current OQMD required ~40M CPU hours to date. Materials Project says ~75M.
- Storage (currently choose not to store all data, i.e., not wavefunctions, some metadata (ELF), etc.)
- Personnel (not only to generate data, but develop interfaces, code)
  - User Friendly Interfaces
- Allocations exist (INCITE, ALCC, XSEDE), however:
    - Code availability
    - Need allocations for high-throughput DFT
    - Need "medium-sized" allocations (e.g., 10^7 hours)

Collaborations/Synergies

- DFT data provides connection to many other working groups
  - CALPHAD – lattice stabilities, formation energies, mixing energies, etc.
  - Materials informatics
    - DFT databases provide large, uniform datasets for ML
    - Informatics can direct DFT to promising compositions – accelerated materials discovery
  - Experimental Data working group – parallel efforts - materials properties already computed or "computable"?
    - Complemented Experimental Efforts (e.g., assist in phase identification),
    - Understanding Materials Behavior, or
    - Guide/predict future experiments
  - Polymers
    - Connections not as straightforward, due to complexities of polymer materials
    - Commonly-used XC not typically suitable for polymers (e.g., vdW, GW)

Collaborations/Synergies

Other NIST collaborations:

- NIST Materials Resource Registry
  - Should register existing DFT databases under MRR (easy)
- DFT Database of Lattice Stabilities
- DFT Diffusion Database
- Collaboration with statistician – quantify uncertainties