Group 2: Tools & Services

Group members:

A. Agrawal (Northwestern U); N. Ferrier (Argonne NL); M. Giovani (U of Chicago); V. Hegde (Northwestern U); W. Joost (DOE); K. McHenry (NCSA); C. Toher (Duke U); J. Warren (NIST); H. Wu (U of WI); M. Zentner (Purdue U)

CHiMaD

What are primary challenges for materials tools & services?

in terms of 1) the materials research community; 2) industry 3) other materials tools and services

- *Materials Research Community*
  - *Representing Methods (missing metadata)*
  - *Avoiding disruption of existing workflows*
  - *Representation of measurement*
  - *Should have incentives*
  - *Benchmark tests for experiment and simulation*
  - *Uncertainties are not being quantified*
  - *Quality assessment tools*
  - *Flexible data models*
  - *Managing expectations across communities*
  - *Diversity of choice and sunk costs*
  - *Updating after share challenges*
- *Industry*
  - *Licensing and the risks GPL*
  - *Weak security models*
  - *Current state of the infrastucture.*
  - *Prior understanding of the likelihood of success (obvious ROI)*
  - *Interested in hearing from Citrine on this*
  - *Distance between industrial practice and cutting edge academic results (particularly in functional materials)*
- *Materials tools*
  - *What about group 4, what do they think?*
  - *Groups should be talking to each other*
  - *Competition versus Collaboration (a role for funding agencies)*
  - *Open versus closed model*

CHiMaD

Key points of Group 2 discussion

- *Materials Research Community*
  - *Outreach / Collaboration*
    - *Represention Methods (missing metadata)*
    - *Representation of measurement*
    - *Licensing and the risks GPL*
  - *Barriers to adoption beyond the computer and materials science*
    - *Avoiding disruption of existing workflows*
    - *Diversity of choice and sunk costs*
    - *Should have incentives besides forcing someone to do it with money*
    - *Competition versus Collaboration (a role for funding agencies)*
  - *Quality*
    - *Benchmark tests for experiment and simulation*
    - *Uncertainties are not being quantified*
    - *Assessment tools*
- *Industry*
  - *Weak security models*
  - *Interested in hearing from Citrine on this*
  - *Distance between industrial practice and cutting edge academic results (particularly in functional materials)*
- *Materials tools*
  - *What about group 4, what do they think? Remit of infrastructure*
  - *Groups should be talking to each other*

CHiMaD

Group 2
proposed low barrier activity

- *Benchmark tests for experiment and simulation*
  - **Phase Field example**
  - **What are "good experiments"**
  - **Multi-flavor DFT comparisons for formation energies**

CHiMaD

Requirements/needs/collaborations to accomplish Group 2 activity

- Leadership (OQMD has graciously volunteered)
- Cookies
- Small amount of glue money