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)
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 infrastructure.
  - 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
Key points of Group 2 discussion

- **Materials Research Community**
  - Outreach / Collaboration
    - Representation 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
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
Requirements/needs/collaborations to accomplish Group 2 activity

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