CHiMaD | Center for Hierarchical Materials Design

NIST/ CHiMaD Workshop Agenda
Data, Databases, & Discovery
Monday, January 25, 2016

All events will be held in the CHiMaD HQ

9.15 am   **Welcome**
Peter Voorhees, James Warren, & Laura Bartolo

9:30 am   **National Data Service & Midwest Big Data Hub**
Ed Seidel (NCSA, NDS, & Midwest BD Hub)

10:00 am   **Materials Data Facility** (30 min)
Ian Foster (Argonne National Laboratory)

10.30 am   **Working Groups finalize previous discussions & steps; begin preparation of 15-minute joint presentation on workshop template for afternoon sessions**

12:00-1:00   **Lunch**

1:00- 2:00   **Working Groups finalize previous discussions & steps; prepare 15-minute joint presentation on workshop template for afternoon sessions**

2.00 pm   **Working Group 1: MDCS, DSpace, MRR & MDF**
Group Presentation & Questions/Comments)

2:20 pm   **Working Group 2: Experimental Data**
Group Presentation & Questions/Comments

2:40 PM   **Working Group 3: Schemas for Polymer Nanocomposite Data**
Group Presentation & Questions/Comments

3:00 PM   **Working Group 4: Natural Language Processing**
Group Presentation & Questions/Comments

3:20 PM   **Working Group 5: DFT**
Group Presentation & Questions/Comments

3:40 PM   **Working Group 6: Building CALPHAD proto-databases**
Group Presentation & Questions/Comments

4:00 pm   Discussions lead by Peter Voorhees & James Warren

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At the Workshop, please use the 2.5-hr working sessions for the WGs to prepare one 15-minute joint presentation about issues, challenges, & proposed next steps

Working Group 1: MDCS, DSpace, MRR & MDF
ANL/UofC: Ian Foster (WG Discussion Leader), Ben Blaiszik
CHiMaD: Laura Bartolo
NIST: Alden Dima, Sharif Youssef, Chandler Becker, Zachary Truatt, Casey Hume, Ray Plante
Possible Areas: NIST Materials Resource Registry & CHiMaD MDF MRR; MDCS DSpace and MDF; metadata in MDF and Registries

Working Group 2: Experimental Data
ANL: Fanny Rodolakis
NIST: Lee Richter, Daniel Sunday, Joe Kline
Northwestern University: Peter Voorhees (ANL), Yip-Wah Chung, Mike Bedzyk, David Seidman, David Dunand, James Coakley, Daniel Sauza, Ding Wen (Tony) Chung
University of Chicago: Paul Nealey (ANL) (WG Discussion Leader); Luping Yu;
Possible Areas: : Explore different data curation methods

Working Group 3: Schemas for Polymer Nanocomposite Data
NIST: Fred Phelan
Northwestern University: Cate Brinson (WG Discussion Leader), Wei Chen, Richard Zhao, Xiaolin Li, Alona Furmanchuk, Yichi Zhang
Possible Areas: Schemas for polymer nanocomposites

Working Group 4: Natural Language Processing & Materials Databases
NIST: Kenneth Kroenlein, Alden Dima; Adele Peskin
University of Chicago: Juan de Pablo (WG Discussion Leader); Roselyne Tchoua
Northwestern University: Alok Choudhary, Ankit Agrawal, Amar Krishna
Possible Areas: Discuss & compare individual natural language processing efforts

Working Group 5: DFT
NIST: Francesca Tavazza (WG Discussion Leader), Ben Burton, Yannick Congo
Northwestern University: Chris Wolverton, Logan Ward, Arindam Paul
University of Chicago/ANL - Giulia Galli, graduate student/post doc
Questek: Jeff Doak
Possible Areas: high-throughput scripts for DFT, electronic transfer calculations; DFT benchmarking,

Working Group 6: Building CALPHAD Proto-Databases
NIST: Carelyn Campbell (WG Discussion Co-Leader); Ursula Kattner; Ken Kroenlein, Guillaume Sousa Amaral
Northwestern University: Greg Olson (WG Discussion Co-Leader), Wei Xiong, Peisheng Wang, Matthew Peters,
Questek: Jason Sebastian, James Saal
Possible Areas: Status on open protodata; Getting data into developing databases