



Kick-off meeting– Oct. 19, 2015
Argonne National Laboratory, A323 Conference Room (Bldg. 241)

- 9:00- 9:15 a.m. Summary of project and meeting objectives – Galli
- 9:00-9:45 a.m. Summary and discussion of **available data for the three main joint experimental-theoretical investigations** and of where data can be found and stored
- Project 1: Assembly of solids of nanoparticles and optimization of their transport properties—Talapin (10 +5)
Project 2: Annealing Processes Out of Equilibrium to Create Nanostructured Multi-Phase Assemblies—Kanatidis (10+5)
Project 3: Interfaces Between Solids and Aqueous Solutions: Optimization of Interfacial Ion Organization—Fenter (10+5)
- 9:45-10:45 a.m. **Software** – where we stand and plans for development & integration
- Qbox and West: Gygi & Galli (15 + 5)
Sages & COPPS: de Pablo & Whitmer (15 + 5)
HOOMD-blue & LAMPPS: Glotzer & de Pablo (15 + 5)
- 10:45-11:00 a.m. Coffee Break
- 11:00-11:30 a.m. Discussion on action/priority items for software development and integration; led by Gygi
- 11:30-12:00 p.m. Discussion on hiring for software development and collaborations (All: please present your plans at the meeting, ideally with name of candidates)
- 12:00- 1:00 p.m. Lunch

- 1:00-2:00 p.m. **Data** organization and simulation environment: what to build
Bair (15+5)
Foster & Wilde (15+5)
Summary of action/priority items for data, led by Bair (20)
- 2:00 -2:30 p.m. Discussion on hiring for data and collaborations, including
web sites, wiki, etc.
(All: please present your plans at the meeting, ideally with name of
candidates)
- 2:30 -3:00 p.m. Coffee Break
- 3:00 -4:00 p.m. **Validation** -- plans for development & integration with theory
(talks below to be coupled theory/expt. Talks for validation
procedure given the available data presented in the morning (9-
9:45) and the plan for future experiments
- Nanoparticles -- Talapin, Lee et al. (10 + 5)
 Interfaces -- Fenter, Olvera dc et al. (10+5)
 Nanocomposites/thermal -- Kanatzidis et al. (10+5)
 Spectroscopy-- Ferrier et al. (10+5)
- 4:00—4:30 p.m. Discussion on action/priority items for validation, including future
seeds (e.g. Lopez)--led by Mitchell
- 4:30—5:00 p.m. Discussion on validation for data and collaborations
- 5:00-5:30 p.m. Discussion of SAB and meeting summary -- Galli