LA-SIGMA Breakout Sessions
Materials for Energy Storage and Generation

Science Challenge

- Principal scientific challenge is multiple-scales: electronic, atomic, microstructure (in space), and collision to transport to function (in time) particularly in the context of nano-structures.
- Integration of molecular dynamics and kinetics with nanofluidic applications (this should impact drug delivery challenge in bio group).

Scientific Collaboration

- Software training: DMOL3, CASSTEP, CP2K, VASP, and AMBER, GROMACS, NAMD, LAMPS and others.
- Large data state questions, curation, data re-use, using many simulation tools coherently.

Diversity, External Engagement, and Workforce Development

- Industrial collaborations/internships should be particularly accessible in this category.
- K-12 demonstrations (*e.g.*, Feynman's heat engine) should be particularly accessible.
- Popular science presentations on "energy and its management" should be particularly accessible. What do you do with wind energy when everyone is sleeping? What happens when everybody plugs-in their car at the same time?
- Visits to out-of-state HBCUs (*e.g.,* Jackson State).

Teaching needs

- Large data set science, data sharing, re-use, curation.
- Nanosystems modeling (existing class at LA-TECH).
- Modeling for experimentalists, nanoscience experiments for modelers.
- PODCASTS & etc: How should these fit with/into classes-for-credit at the different universities?
- Project could have a play-list of contributors, expertise, topical presentations for reuse at the different locations.