LA-SIGMA Breakout Sessions
Massively Parallel DFT and Force Fields

Science Challenge

Main challenges:

To expand the system size of what can be examined, and to span the conditions, such as interfaces, defects, and nanostructured materials.

To develop fully non-local correlation functionals capable of describing electronic materials.

1) Ab Initio calculations on atom clusters with high spin states.
2) Periodic DFT to investigate larger systems, interfaces, and defects
3) Force field that can accurately reproduce 1) and 2), that is simple enough to be widely used and combined into general simulation codes, and is transferable over multiple conditions.

Scientific Collaboration

Help create the tools to be used by the energy storage science group.

Create the tools to be used by highly correlated materials.

Collaborate with cyber infrastructure to store some of the DFT results to be used for force field development, and also work with them to help develop modules to carry out the calculations necessary to fit force fields; workflow software tools.

Diversity, External Engagement, and Workforce Development

Provide new molecular models and density functionals that will be used by the greater scientific community.

These tools will be made available for industrial companies to calculate properties of new catalysts

Integrate these into existing molecular dynamics codes, such as LAMPPS

Teaching needs

A new course will be developed focusing on DFT calculations of materials that will be somewhat adapted from the course taught at Tulane by John Perdew, “Atomic and Molecular Physics”. This course will also include aspects about atomic force fields, and will be made available for all institutions.