Fundamental Interactions and Energetics in Ferroelectric Materials

M. Uludogan, T. Cagin
Department of Chemical Engineering
TAMU

Objectives

- Using state of the art simulation and modeling methods to understand behavior and properties of materials as a function of
  - Chemical constitution
  - Composition
    - through various processing approaches
  - Structure
    - role of nano- and micro-structure the nanostructure through processing

  for improving their performance for engineering application
- Use and develop simulation and modeling approaches to elucidate mechanisms, and optimum parameters for processing materials with better performance.

Simulation Method Used

- Density Functional Theory
  - Vienna Ab-initio Simulation Package (VASP)
    - Plane Wave Code
    - Periodic Boundary Conditions
    - US PP+ PAW potentials (low energy cut-off)
    - MPI (serial +parallel)

Runs

- Batch system
  - 32 cpu mpi (< 24 hours)
    - 40-50 atoms (static force calc.)
  - 64 cpu mpi (< 12 hours)
    - 40-50 atoms (low symmetry calc)
    - 70-80 atoms (high symetry)
  - 128 cpu mpi (< 6 hours)
    - 320 atoms (static calc.)

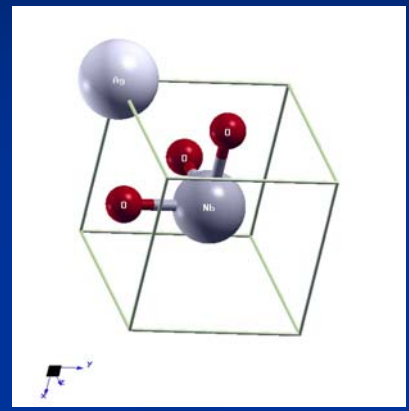
Computation Requirements

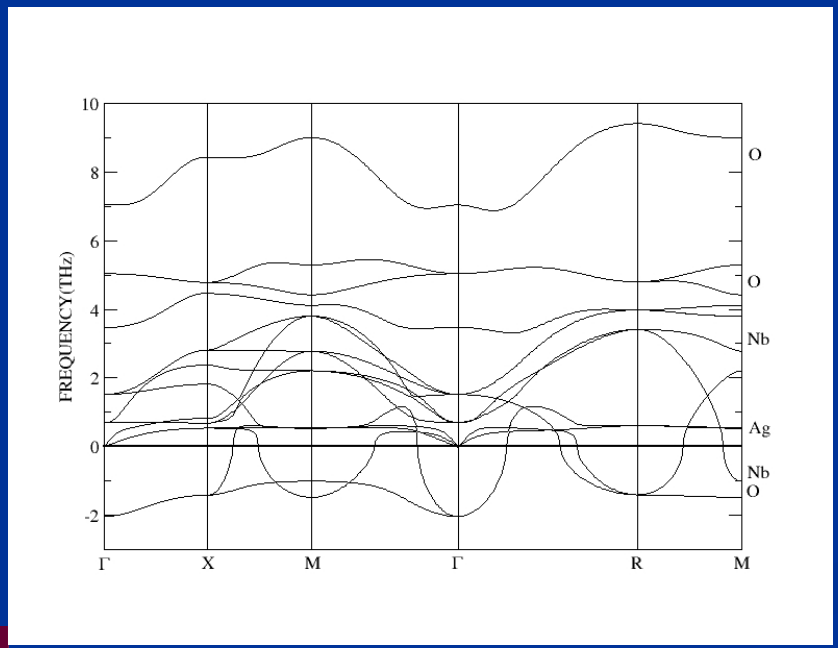
- Methodology related
  - Frequency spectrum (phonon) calculations
    - Linear Respose (Pert. Theory)
    - Direct Method (Finite Diff. of forces)
      - 5-10-40 atom unit cells
      - 2x2x2 supercells (40-80-320 atoms)
- Resources related
  - Adjusting simulations to available resources
    - Decreasing memory demand
    - Decreasing precision and cpu

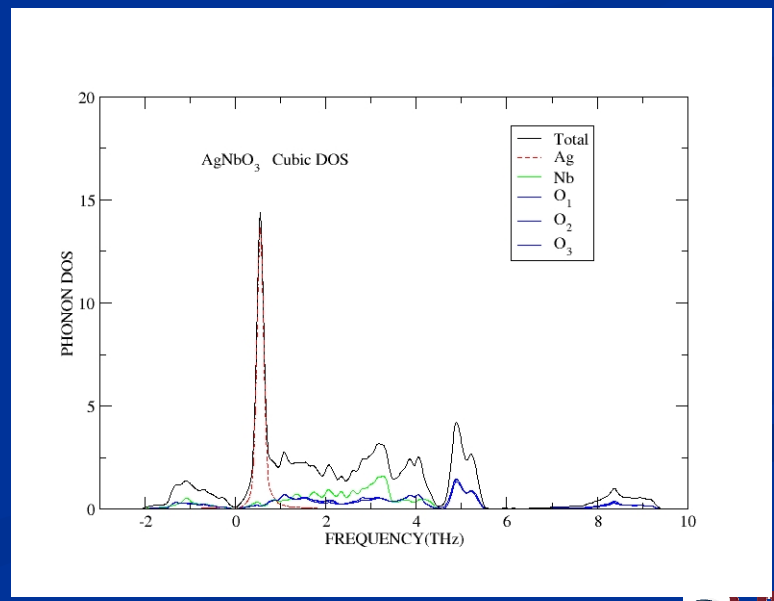
Comparison with other architectures

- Focus : Speed + stability
- No real time comparison
- Resource demanding problems

$AgNbO_3$







Future Use

- Main queues
  - 32mpi
  - 64mpi
  - 128mpi(low symmetry + large supercell)