



- Comparisons of total system energy for six **triclinic** systems with identical initial conditions, computed using the June 17, 2013 version of LAMMPS.
- Trajectories include 405,000 time steps of velocity selection/NVT equilibration, followed immediately by 2,000,000 time steps using NVE integration.
- Energy is conserved when long-range terms are computed using the ewald method, but not ppm, with accuracy set to 10^{-6} .
- Titles indicate k-space solver, real-space cutoff for both coulomb and dispersion, and pair style used.
- Pair styles are BCCL = buck/coul/long and BLCL = buck/long/coul/long.
- These figures are reproducible across two different machines builds of LAMMPS from two different compilers (mpicc and mpic++).