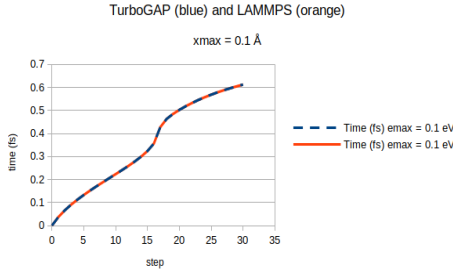
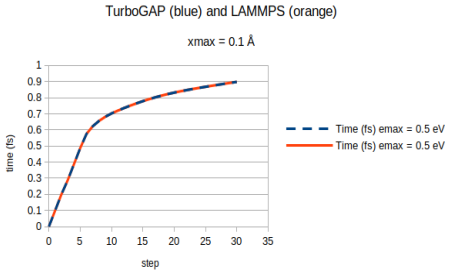
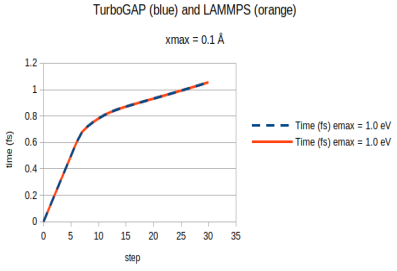
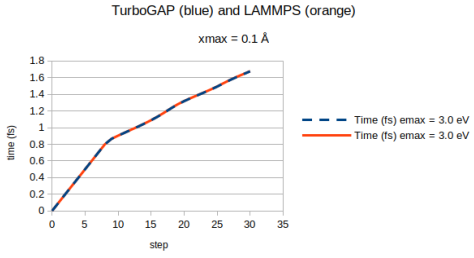
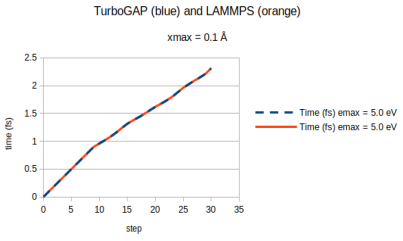
Binary Collision Simulations using TurboGAP and LAMMPS and sensitivity of time step to xmax and emax criterion

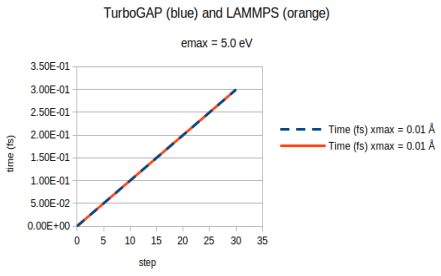


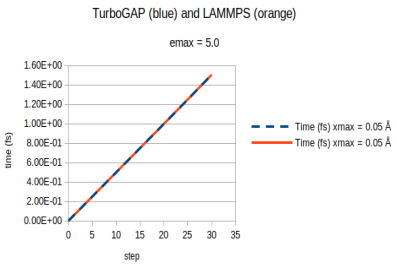


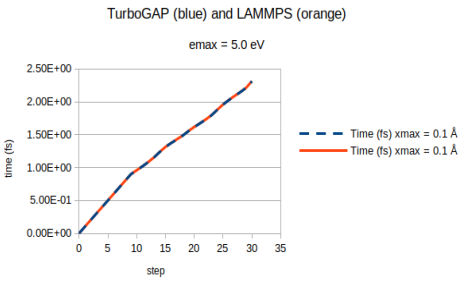


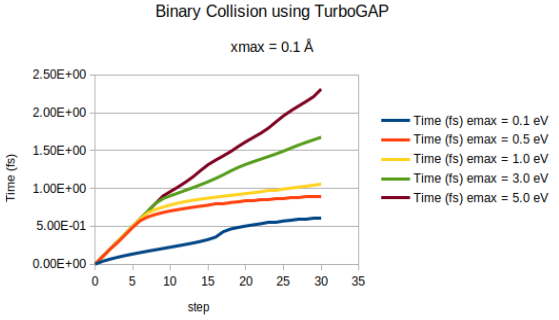


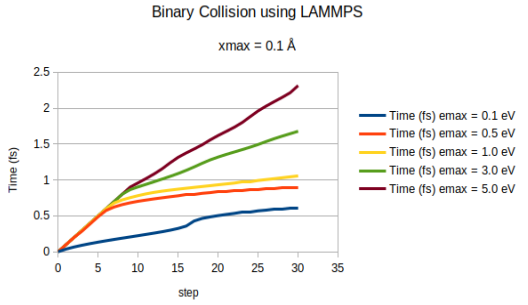


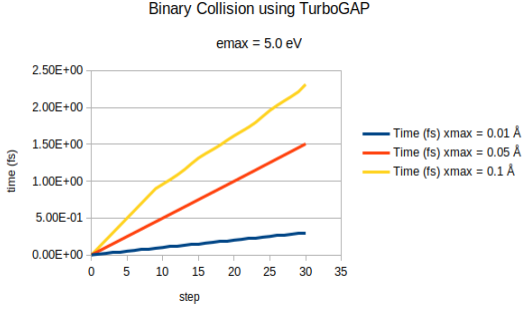


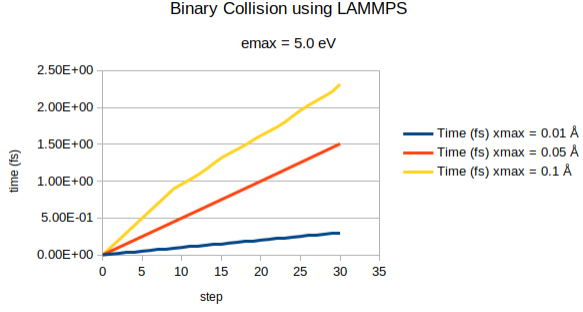












Two Si atoms
at r_1 = (10.0, 10.0, 10.0) and r_2 = (13.0, 10.0, 10.0)
with v_{1x} = 1.0 Å/fs, v_{1y} = 0.0, v_{1z} = 0.0 and v_{2x} = -1.0 Å/fs, v_{2y} = 0.0, v_{2z} = 0.0
using Si (not stiffened) GAP potential.

Full EPH model in TurboGAP and LAMMPS

216 Si atoms in a box of dimensions 16.29 Å on each side.
Using Si-GAP potential.

Ta = 0.0 K, Te = 300.0 K
Coupling parameter – constant case
T. Jarrin et al. Phys. Rev. B 104, 195203
$C_e = 3.5*10^{-6}$ eV/K/Å^3
$K_e = 0.1248$ eV/K/Å/ps