

ChE 548
Take-Home Midterm
due 8:00 a.m. Monday, March 14, 2005
Spring, 2005

Perform a molecular dynamics simulation of F_2 at $T = 500$ K and $p = 1$ atm. Report the density, the potential energy, pressure, and self-diffusivity. Where available report standard deviations. Report the values of r_{cut} , n_{br} , max_{eqb} , max_{stp} , N , and Δt that you used. Verify that the simulations are long enough to generate the infinite-time limit dependence of the mean square displacement in the Einstein relation. Use an appropriate method from Chapter 17 of BSL2 to generate a theoretical value for the same system.

This is a midterm examination. No communication between classmates is acceptable. If it is determined that two or more students worked together on this exam, then all students involved will receive zeros for the exam.