Exam 1
ChE 548
Spring, 2007

**Problem 1.**
Based on the results of Homework 3, answer the following questions.
(a) In an MD simulation, does it take longer for a gas or liquid phase to reach the Einstein infinite time limit in order to get a good diffusivity?
(b) Based on your reasoning in (a), will it take longer for a simulation to reach the Einstein infinite time limit at low or high temperature?
(c) In a binary mixture, which component will have the higher self-diffusivity, the one with the higher or lower molecular weight? Why?
(d) In a binary mixture, which component will have the higher Fickian diffusivity, the one with the higher or lower molecular weight? Why?
(e) What's the general rule for the minimum number of molecules in an MD simulation?

**Problem 2.**
The corresponding states charts for shear viscosity, thermal conductivity and self-diffusivity appear on pages 22, 272 and 522 respectively of BSL2.

(a) Report the trends in shear viscosity, thermal conductivity and self-diffusivity as a function of temperature for the *ideal gas* based on the corresponding states chart, e.g. do these properties increase or decrease with temperature?
(b) Equation (1.4-8) on page 24, (9.3-11) on page 275 and (17.3-8) on page 526 provide estimates from kinetic theory on the temperature dependence of the shear viscosity, thermal conductivity and self-diffusivity as a function of temperature for the ideal gas. Do these equations provide the same temperature trends as the corresponding states chart in part (a)?
(c) Are all trends with respect to temperature the same for shear viscosity, thermal conductivity and self-diffusivity of the *ideal gas*?
(d) What is the molecular basis for the trends observed in part (a)?

(e) Report the trends in shear viscosity, thermal conductivity and self-diffusivity as a function of temperature for the *liquid* based on the corresponding states chart, e.g. do these properties increase or decrease with temperature?
(f) Equation (1.5-11) on page 31, (9.4-3) on page 279 and (17.4-5) on page 529 provide estimates from a mixture of theory and empiricism on the temperature dependence of the shear viscosity, thermal conductivity and self-diffusivity as a function of temperature for the *liquid*. Do these equations provide the same temperature trends as the corresponding states chart in part (e)?
(g) Are all trends with respect to temperature the same for shear viscosity, thermal conductivity and self-diffusivity of the *liquid*?
(h) What is the molecular basis for the trends observed in part (e)?