**Homework 2: Computational Design of Materials**

Due: Nov 5, 2012

1. A R&D engineer was asked to develop a polymer adhesive for bonding two ITO-coated glass substrates together with long-term reliability. After a preliminary study, he/she selected the following polymers for further screening for their adhesive properties to ITO-coated glass substrate. The polymers are (a) Polyethelene, -[CH2-CH2]$_n$-, with a mass density of ρ=0.94 g/cc; (b) Polystyrene, -[CH2-CHPh]$_n$-, $\rho$ =1.05 g/cc; and (c) Poly(p-nitrostyrene) -[CH2-CHPhNO2]$_n$-, ρ=1.1 g/cc; and (d) Poly(methyl methacrylate) -[CH2-CMeCOOMe]$_n$-, ρ=1.17 g/cc. Can you help to select an appropriate candidate for this application based on the adhesive energy results of Molecular Dynamics simulation?