Abstract Submitted
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Effects of Impurities on the Optical Properties of Mixtures DAN HORNER, JOEL KRESS, LEE COLLINS, Los Alamos Nat. Lab. — We perform molecular dynamics simulations[1] of mixtures of CH_2 and Aluminum (Al) in a plane-wave, finite-temperature density functional theory treatment at the generalized-gradient level with projector-augmented wave pseudopotentials for temperatures between 1eV and 3eV and densities ranging from 1 to 3 g/cm^3. In this regime, the system generally takes the form of an atomic liquid with the C, H, and Al all dissociated. We vary the concentration of Aluminum from 0% to 100% by substituting Al atoms for a CH_2 molecules in the initial configuration. Samples consisted of 75 CH_2 molecules [C=75; H=150] or their equivalent Al substitution although larger samples were introduced to test size effects. In general, the dc electrical conductivity varied smoothly with Al concentration with a slow increase up to 50% and a steeper rise after about 70%. The Rosseland Mean Opacities also behaved smoothly with a factor of two change between the extremes of the Al concentration. However, for a few combinations of density, temperature, and Al concentrations, we did find a "condensation" into a large polymer structure and noticeable changes in the system properties.

[1]D.A, Horner et. al., Phys. Rev. B **80**, 024305 (2009)

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