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.


Lee Collins  
Los Alamos Nat. Lab.

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