338d Thermophysical Properties of Gas Expanded Liquids

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Gas expanded liquids (GXLs) are a new class of tunable solvents which take advantage of the solvent strength of conventional organic liquids combined with the attractive properties of supercritical fluids. GXLs utilize the high solubility of gaseous CO_2 in organic solvents resulting in a highly tunable solvent, at sub-critical pressures. GXLs have recently been applied to gas anti-solvent methods of crystallization and separation, as well as creating tunable solvent environments for reactions. This study investigates the thermodynamic and transport properties of GXLs by a wide range of experimental methods including spectroscopic methods, molecular dynamics simulation and neutron scattering. Comparison of the local environments of solute probe molecules versus bulk solvent properties demonstrate the unique properties of GXL's as a solvent / reaction media. Specific interactions within the media impact the structure and solvent properties are also investigated and provide a synergism between experiment and computation. Further understanding of the tunable thermophysical properties of GXL's is necessary for the application of these fluids for novel reactions and separations.