

Understanding and Controlling Fractional Free Volume in Ionic Liquids, Organic Solvents and Membranes for CO₂ Capture

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Fractional free volume (FFV) is an important physical property that can be correlated to both gas solubility and diffusion in liquid and polymer phases. For conventional organic molecules and solvents, FFV can vary widely, but there is little opportunity for it to be controlled in a rational manner. For systematically variable materials such as ionic liquids (ILs), FFV can be shown to be strongly connected to molecular structure and thus can be tuned/optimized. We have conducted broad surveys of FFV in ILs using COSMOtherm, as well as for imidazoles and many other molecules. As such, a fundamental understanding of the structure-property relationships governing FFV can be determined. Furthermore, the ability to study theoretical ILs and other molecules within COSMOtherm can help identify new synthetic targets by which to control and improve material performances for CO₂ capture and other applications. This talk will focus on integrating the concept of FFV within Regular Solution Theory, the implications for ILs and other molecules, and new synthetic targets that have been identified that can exhibit superior properties.