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A functional approach to solubility parameter computations

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Solubility parameter methods have proven very useful in an array of theoretical and practical applications. From an applications standpoint, solubility parameters are a practical and convenient way to evaluate polymer solubility in organic solvents, as well as the miscibility of semiconductor polymer-polymer and polymer-nanoparticle blends. With respect to more fundamental sciences, correlations between solubility parameter methods and well-known thermodynamic and molecular theories have contributed to our understanding of significant physicochemical system properties, solvent-solute affinities, equilibria, and the development of quantitative structure-property relationships, and phase separation behavior in polymer-based materials. The determination of solubility behavior and solubility parameters represents a challenging mathematical problem of locating the central tendency of solvent affinity based on a limited set of data taken from experimental observations. The most widely used method for computing this central tendency employs a binary classification of solvents, i.e., a solvent is either a good or poor solvent, and constructs an ellipsoidal compatibility region in a three-dimensional Hansen solubility parameter (δD, δP, δH) space. Employing a binary classification requires an arbitrary solubility threshold and an ellipsoidal fitting model imposes a symmetry on the intermolecular forces that is rarely reflected by the experimental data, thereby resulting in as a loss of important information regarding the nature of the intermolecular interactions between the solvent and solute. To overcome these issues, an approach that makes use of accurate solubility data to construct a three-dimensional solubility function, f, is presented. The principles of the approach are discussed in detail and the procedures for generating the solubility function and solubility parameters are described using PCBM solubility data available in the literature. Lastly, a method that employs f as a predictor of solubility in unknown solvents with a proposed measure of reliability is presented.

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