Steve Lustig

Associate Professor
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Steve Lustig joined the Department of Chemical Engineering at Northeastern University as an associate professor in September 2016. Before moving to Boston he was an adjunct professor at the University of Delaware in the Department of Chemical and Biomolecular Engineering and the Department of Materials Science and Engineering, where he taught statistical thermodynamics, polymer physics and green engineering for 8 years. He was a principal investigator at the DuPont Central Research & Development laboratories at Experimental Station in Wilmington, Delaware for 26 years. In 2013 he was awarded the AIChE Industrial Research & Development Institute Award for his work at DuPont. In his spare time he enjoys welding metal sculpture and sailing with his family.

Thermochemical Design for Chemical and Materials Engineering

Abstract

Many design problems in engineering and materials science can be cast in terms of finding molecular structures and mixtures that satisfy thermodynamic criteria. Such common criteria, e.g. binding energy, solubility and partitioning, frequently demand selectivity among components in a mixture. Engineers using molecular modeling to solve these design problems typically proceed in the same, forward fashion as Edisonian experimentalists. Structures are guessed, properties are predicted and the results are compared to the desired outcomes. Learning from the outcomes, this loop is iterated until the results match the desired outcome. In contrast, a direct design method allows the engineer to derive the required molecular structure(s) starting with only the desired properties. Direct computational design may be the best approach when Edisonian trial and error testing is not feasible. Furthermore direct design methods may be faster and provide new molecular structures, previously unknown to the engineer.

COSMOdesign is a new direct design methodology to derive optimal compounds or molecular structures that satisfy specified bounds on thermodynamic properties. The method is based on performing genetic Monte Carlo transformations on the solvation surfaces of molecules under design. The solvation surface provides a simple, two-dimensional surface from which thermodynamic properties can be calculated and appropriate chemical structures can be derived. The evolution of mutations enables the engineer to both assess the opportunity for improving further the design as well as identify the improved molecular structure(s). This methodology has been applied to the design of solutions to many industrial problems involving gas-liquid, liquid-liquid and solid-liquid inverse problems to accelerate the development of green products and processes. The COSMOdesign methodology is illustrated in an example optimization of ionic liquids for more efficient refrigeration based on absorption cooling. Ionic liquids form a broad class of solvents which can often be applied to develop green processes. However, the diversity of options for charge centers, chemical group functionality, valency and molecular configuration presents the most significant obstacle to their selection.

Tuesday February 21st, 2017 | 2112 Learned Hall | 10:00 – 10:50AM