Molecular Modeling and Simulation: Present and Future Tools for Physical Properties Prediction and Molecular Product Design

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Molecular simulation and computational chemistry are powerful tools for understanding and predicting thermophysical properties in systems both at equilibrium and away from equilibrium, and in systems composed of molecules ranging in complexity from spherically symmetric monatomic molecules to polymers. The continuing exponential growth in the speed of computers, combined with advances in massively parallel supercomputing, will result in molecular-based simulation of systems modeled to a high degree of accuracy becoming an equal partner with experiment for the prediction of thermophysical properties for industrial purposes.

In this presentation, the current capabilities of molecular modeling tools for thermophysical properties prediction and molecular-based product design will be briefly reviewed. In addition, the prospects for further progress in this area in the next decade and beyond will be assessed. As molecular-based product design becomes a practical reality, process design will be affected in myriad ways, ranging from the ready availability of otherwise-unattainable data in physical properties databases to the prospect of simultaneous product/process design to meet demanding performance specifications and/or environmental regulations.