Integration of Thermodynamic Properties from Different Databases with Data Derived from DFT and Ab-Initio Methods, and Their Delivery Through Web Services

Christophe Paolini and Himen Jain
Computational Thermodynamic Laboratory, Mechanical Engineering Department, San Diego State University, San Diego, CA, U.S.A.

Subrata Bhattacharjee [C, S]
Mechanical Engineering Department, San Diego State University, San Diego, CA, U.S.A.

While the JANAF tables, NIST Webbook, and NASA database are well known as reliable sources for thermophysical data, they do not always agree completely. For example, the specific heat of nitrogen dioxide from these sources shows significant discrepancy over a large temperature range. Also, data on some species may be incomplete or absent. In this work, we extend a Web Service based infrastructure called CHEQS, developed at San Diego State University, that allows users to 'plug-in' existing data from different sources into their specific applications. Users can switch among different data sources and evaluate the impact of data on their applications. It also allows users to compute thermophysical properties using DFT and various ab initio methods at different levels of theory. The computed data then can be fitted to a standard model such as the Shomate polynomial used by NIST and can be integrated into CHEQS. A simple example is presented using Benzoic acid, commonly used as a thermodynamic standard in bomb calorimetry, for which data is incomplete in the NIST Webbook. Using DFT, thermophysical properties of Benzoic acid were calculated at different temperatures and then fitted to produce the coefficients of the power series used in NIST and NASA thermophysical databases. The impact of choosing different data sources is evaluated by calculating the chemical equilibrium composition of propane combustion at different equivalence ratios. Equilibrium computation is performed by a Java applet running in a web browser in which a user selects a particular source, and the corresponding data is retrieved from CHEQS through a Web Service call before computations are performed.