Predicting the properties of materials: Stepping into the unknown

To use a material, one needs to know and understand its properties – its density, its hardness, its strength, etc. – and the relation of the relevant properties to the desired application. Those properties listed above are accessible to simple empirical observation, while other important properties require detailed experimental measurement: for example, the combination of materials able to form the material; the energy required in its preparation; its stability against changes in temperature or pressure; its resistance to degradation; and so forth.

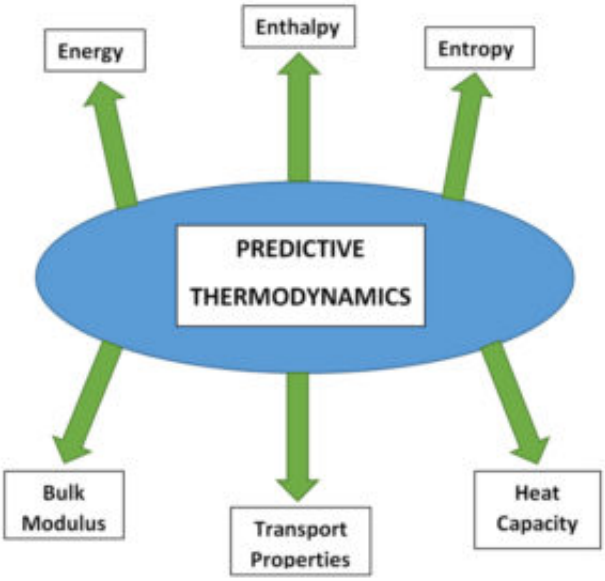

Fig. 1.

There is no way in which all properties can have been measured for each of the innumerable materials available for our choosing, while myriad new materials are continually synthesised or even hypothesised. For these reasons, predictive methods are increasingly necessary. Over the years numerous property predictive methods have been developed with names such as: property correlations, group contribution methods, quantitative structure-activity relations (QSAR), molecular mechanics, quantum mechanics, and many others. One important area for property investigation is related to energy, which is the subject of Thermodynamics. This is an especially problematic area since thermodynamic measurement requires both expertise and equipment, so demanding reliable predictive methods to supplement and even check experimental measurement.

We, together with our colleagues and others, have noted that many energy-based properties are related to the molar volume (that is, to the volume occupied by a mole of the material) or, similarly,

to the density of the material – this appears to be based on the fact that the atoms and ions making up a material are in intimate contact, so that changing volume results in changing the energetic interactions. Furthermore, the molar volume is itself accessible to prediction!

We have developed procedures for ionic materials which we term Volume-Based Thermodynamics (VBT) where we relate many properties to the molar volume of the material. For example, entropy is observed to be proportional to molar volume – which is important since entropy controls the temperature-dependent behaviour of materials. Similarly, the energy involved in the formation of a material is directly related to the mean distance between ions, and so also to its molar volume.

Another important relation that we use is a Thermodynamic Difference Rule (TDR) which notes that substitution of one ion by another with similar characteristics produces changes in the thermodynamic properties which are related to the size of the ion.

The application of these relations requires access to data by which correlations to volume, or among other properties, can be established. It is fortunate that there are many thermodynamic databases on which this work can be based. Correspondingly, the investigator who requires property knowledge can use such databases together the established correlations to predict the properties that are required. These techniques have been applied to such diverse materials and conditions as to minerals, to ionic liquids (an area of current importance since they constitute environmentally friendly solvents), to explosive materials, to conditions in outer space and in the interior of the planets, to energy storage, and so forth.

Thermodynamic predictive methods permit the investigator to use his/her imagination in applying materials.

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