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BOOK REVIEWS

Molecular Theory of Water and Aqueous Solutions, Part I: Understanding Water. By Arieh Ben-Naim (The Hebrew University of Jerusalem, Israel). World Scientific, Ltd.: Singapore. xxx + 629 pp. $98.00. ISBN 978-981-283-760-8.

Scientists involved in computer modeling of liquid water and biological materials should find this volume useful. It has 478 references to the literature, of which 51 are by the author. This book gives a reasonable coverage of the computational side of the study of liquid water, with emphasis on low dimensional, nonquantum mechanical models.

Truly understanding water is no small task. Einstein is quoted as saying that if he could get only one set of data from a material he would want the heat capacity, C_p. It is telling that this piece of information that has been in the literature for years is only partially available in this reference book. The heat capacity data that are missing from the volume are those for the liquid below 0 °C (see C. A. Angell, M. Ogunl, W. J. Sichina, *J. Phys. Chem.* **1982**, *86*, 998−1002). These data are essential for understanding the properties of liquid water and have not been satisfactorily modeled by any of the multidimensional mixture models discussed in the book. Figure 1.25 is a display of the values of C_p, as a function of pressure from 1 to 1000 atm (0.10 GPa). The author then concludes that, under conditions of high pressure (0.05 GPa or higher), water is a normal liquid. This conclusion ignores all of the solid work that has been done on the putative second critical point for water. It also ignores the published work on the PVT surface of liquid water, which shows that C_p for water must increase at a pressure of 0.1 GPa at temperatures below 288 K (see O. Mishima, H. E. Stanley, *Nature* **1998**, *392*, 164−168). The requirement for the increase in C_p stems from the anticipated increase in volume of the liquid and Ben-Naim's principle correlating increases in binding energy with decreases in density for liquid water.

Solvation and solutions are a very broad and complex set of topics for liquid water. Ionic solutions are largely ignored in the treatment presented here, though substantial ground-breaking work has recently been done on this subject (see, for example, J.-J. Max, M. Trudel, C. Chapados, *Appl. Spectrosc.* **1998**, *52*, 234−239 and more recent publications by C. Chapados). Hydrophilic interactions are said to be "far more important in biochemistry" in the Preface. Treatment of solvation of simple ions like Cl^- in water seems to be missing from the book. Hydrophobic solutes are extensively covered, with particular attention to treatments developed by the author.

This volume is an elegant presentation of a statistical mechanical approach to liquid water. To the extent that it succeeds in that arena, it is valuable. However, the utility of the book for a general reader with a chemical physics background and interests may be limited by the intense focus of the work on statistical mechanics and the areas where its results correlate with the properties of water.

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