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Introduction: Water

Water is the most important liquid material known and probably the most important material. H_2O is the most important biomolecule and maybe the most important molecule. We do not study only materials that are definably important, and this observation cripples these argumentative but defensible propositions. Interesting materials, important enough to justify sophisticated molecular research, are everywhere. Nevertheless, it is difficult to overestimate the importance of water materials in our science, history, and culture.

Water has been around. Water *is* a material with a biography (Ball, P. *Life's Matrix: A Biography of Water*; Farrar, Straus and Giroux: New York, 1999.) if not a criminal record. Treatises (Franks, F. *Water: A Comprehensive Treatise*; Plenum: New York, 1973; Vols. 1−7.) and monographs (Eisenberg, D.; Kauzmann, W. *The Structure and Properties of Water*; Oxford University Press: New York, 1969. Robinson, G. W.; Zhu, S.-B.; Singh, S.; Evans, M. W. *Water in Biology, Chemistry, and Physics*; World Scientific: Singapore, 1996.) chronicle its peculiarities. In contrast to research directed toward discovery of exotic new materials, objective veracity of a molecular scale understanding is often a primary goal of research on aqueous materials. The importance and ubiquity of aqueous materials often complicates this goal. However, the challenges of a quantitative understanding of water materials of a molecular scale are well recognized if not entirely well solved.

The breadth and intensity of the continuing study of water typically surprises researchers on other topics because water is so commonplace to our experience. However, aqueous materials are anomalous in the broad field of other liquids and solids. In contrast to many other solvents, for example, liquid water can be viewed as a *chemical* liquid in that it not only provides a medium for solution chemistry but often participates in elementary chemical events on a molecular scale. Yet the water molecule is among the simplest. The basic question of precisely how this simplicity leads to the complexity of the materials we know continues to challenge and fascinate researchers on water and aqueous systems.

Because the basic raw ingredient of aqueous materials is so common, topical problems are often defined by juxtaposition of some other interesting topic with the ubiquitous water matrix, so with molecular biology, biotechnology, nanotechnology, and topics of mineralogy and oceanology in Earth sciences. These are frequently subjects that involve specialized research on water.

Despite the commonality and because of the importance and complexity, new measurements and new ideas on aqueous materials continue to startle this research field. The reviews in this thematic issue of *Chemical Reviews* on Water represent several of the recent surprises. C. A. Angell reviews "Liquid Fragility and the Glass Transition in Water and Aqueous Solutions". Beyond the intellectual puzzles posed by aqueous glasses, interest here is supported by the observation that most of the condensed water in the universe is probably present as glassy materials on interstellar grains and by the practicalities of cryopreservation of materials of biological origin. T. Head-Gordon and G. Hura review recent progress in scattering studies of atomic pair correlations in liquid water. They also discuss the performance of current force field models with reproducing the present experimental information on those pair correlation functions. The succeeding review of L. R. Pratt and A. Pohorille overlaps and complements this aspect but from the perspective of aqueous interfaces of potential biophysical interest. The modeling of aqueous interfaces is topical because surprising recent progress in understanding hydrophobic effects on a molecular scale has renewed interest in hydrophobic effects in macromolecular and interfacial settings. Recent experimental studies of aqueous interfaces on the basis of vibrational sum frequency spectroscopy are reviewed by G. L. Richmond. This work is providing new information on aqueous surfaces and is applicable to interfaces of impressive complexity. Again, Pratt and Pohorille, reviewing the theoretical side of some of these problems, provide some complementarity to the discussion of Richmond.

The paper titled "Roles of Water for Chemical Reactions in High-Temperature Water" by N. Akiya and P. E. Savage provides an illustration of the view suggested above that water is, relative to many alternatives, a peculiarly chemical solvent. The variety of issues that come up (see Table 3) and the importance of these topics is again notable. The later paper of U. M. Lindström reviews water-based or-

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ganic synthesis. In reviewing measurements of enthalpies and entropies of transfer for ions between water and mixed aqueous−organic solutions, the paper by G. Hefter, Y. Marcus, and W. E. Waghorne underscores points that are not emphasized frequently enough: thermodynamic data affect quantitative molecular theories and modeling calculations at 100% efficiency; each datum makes a difference. This is due naturally to the quantitative focus of such results. An additional simplistic interpretation that might water down the truth content is not required in order for thermodynamic experiments to be acceptable; a correct value is enough. The broad topic of speciation of ionic materials dissolved in water is important and often complicated. The final paper in this issue, "Fate of Fluorosilicate Drinking Water Additives" by E. T. Urbansky, reviews a specific topical segment of that broad area.

The combination of work discussed in this collection gives a helpful impression of the scope of current work. Other special collections of research reports on liquid water and aqueous solutions (Soper, A. K.; Rossky, P. J. *Chem. Phys.* **2000**, *258*, 107−108.) complement the comprehensive reviews found in the present issue.

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