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Fall 2017 Physics Newsletter

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New Developments in Gastrointestinal Imaging

C-H Activation in Organic Synthesis (CHAOS), as a MC member from Malta [CA15106 MT].

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J.E. Enderby At the last NATO-ASI on liquids held in Corsica, (August 1977), Professor de Gennes, in his summary of that meeting, suggested that the next ASI should concentrate on some specific aspect of the subject and mentioned explicitly ionic solutions as one possibility. The challenge was taken up by Marie-Claire Bellissent-Funel and George Neilson; I am sure that all the participants would wish to congratulate our two colleagues for putting together an outstanding programme of lectures, round tables and poster session. The theory which underlies the subject was covered by four leading authorities: J.-P. Hansen (Paris) set out the general framework in terms of the statistical mechanics of bulk and surface properties; H.L. Friedman (Stony Brook) focused attention on ionic liquids at equilibrium, and J.B. Hubbard considered non-equilibrium properties such as the electrical conductivity and ionic friction coefficients. Finally, the basic theory of polyelectrolytes treated as charged linear polymers in aqueous solution was presented by J.M. Victor (Paris).

The study of intermolecular forces began over one hundred years ago in 1873 with the famous thesis of van der Waals. In recent decades, knowledge of this field has expanded due to intensive research into both its theoretical and the experimental aspects. This is particularly true for the type of very strong cohesive force stressed in 1920 by Latimer and Rodebush: the hydrogen bond, a phenomenon already outlined in 1912 by Moore and Winemill. Hydrogen bonds exert a profound influence on most of the physical and chemical properties of the materials in which they are formed. Not only do they govern viscosity and electrical

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conductivity, they also intervene in the chemical reaction path which determines the kinetics of chemical processes. The properties of chemical substances depend to a large extent on intermolecular forces. In spite of this fundamental fact, too little attention is given to these properties both in research and in university teaching. For instance, in the field of pharmaceutical research, about 13000 compounds need to be studied in order to find a single new product that can be successfully marketed. The recognition of the need to optimize industrial research efficiency has led to a growing interest in promoting the study of intermolecular forces. Rising salary costs in industry have encouraged an interest in theoretical ideas which will lead to tailor made materials.

As the various disciplines of science advance, they proliferate and tend to become more esoteric. Barriers of specialized terminologies form, which cause scientists to lose contact with their colleagues, and differences in points-of-view emerge which hinder the unification of knowledge among the various disciplines, and even within a given discipline. As a result, the scientist, and especially the student, is in many instances offered fragmented glimpses of subjects that are fundamentally synthetic and that should be treated in their own right. Such seems to be the case of the liquid state. Unlike the other states of matter -- gases, solids, and plasmas -- the liquid state has not yet received unified treatment, probably because it has been the least explored and remains the least understood state of matter. Occasionally, events occur which help remove some of the barriers that separate scientists and disciplines alike. Such an event was the ASI on The Liquid State held this past July at the lovely Hotel Tivoli Sintra, in the picturesque town of Sintra, Portugal, approximately 30 km northwest of Lisbon.

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Since this broad a subject could not be covered in one Institute, the focus of the ASI was on a theme that provided a common thread of understanding for all in attendance -- the Electrical Properties of the Liquid State.

Freeze-drying, or lyophilization, is a well established technology used in the preservation of numerous pharmaceutical and biological products. This highly effective dehydration method involves the removal of water from frozen materials via the direct sublimation of ice. In recent years, this process has met with many changes, as have the regulations

Generalized van der Waals Theory of Molecular Fluids in Bulk and at Surfaces presents successful research on the development of a new density theory of fluids that makes it possible to understand and predict a wide range of properties and phenomena. The book brings together recent advances relating to the Generalized van der Waals Theory and its use in fluid property calculations. The mathematics presentation is oriented to an audience of varying backgrounds, and readers will find exercises that can be used as a textbook for a course at the upper undergraduate or graduate level in physics or chemistry. In addition, it is ideal for scientists from other areas, such as geophysics, oceanography and molecular biology who are interested in learning about, and understanding, molecular fluids. Presents an approximate, but fully derived and physically explained, theory of molecular fluids to facilitate broad applications Derives a density functional theory of classical fluids and applies it to obtain equations of state, as well as non-uniform fluid properties, e.g., surface tension and adsorption Demonstrates how the theory can be applied to complex multi-center molecules forming a

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polymer fluid Provides user-friendly programs to redraw figures for variable parameters and to perform calculations in particular applications Includes a set of exercises to support use of the book in a course

The aim of this book is to provide the reader with a modern presentation of ionic solutions at interfaces, for physical chemists, chemists and theoretically oriented experimentalists in this field. The discussion is mainly on the structural and thermodynamic properties, in relation to presently available statistical mechanical models. Some dynamic properties are also presented, at a more phenomenological level. The initial chapters are devoted to the presentation of some basic concepts for bulk properties: hydrodynamic interactions, electrostatics, van der Waals forces and thermodynamics of ionic solutions in the framework of a particular model: the mean spherical approximation (MSA). Specific features of interfaces are then discussed: experimental techniques such as in-situ X-ray diffraction, STM and AFM microscopy are described. Ions at liquid/air, liquid/metal and liquid/liquid interfaces are considered from the experimental and theoretical viewpoint. Lastly some dynamic (transport) properties are included, namely the self-diffusion and conductance of small colloids (polyelectrolytes and micelles) and the kinetics of solute transfer at free liquid/liquid interfaces.

Recently there have been profound developments in the understanding and interpretation of liquids and soft matter centered on constituents with short-range interactions. Ionic soft matter

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is a class of conventional condensed soft matter with prevailing contribution from electrostatics and, therefore, can be subject to possible long-range correlations among the components of the material and in many cases crucially affecting its physical properties. Among the most popular representatives of such a class of materials are natural and synthetic saline environments, like aqueous and non-aqueous electrolyte solutions and molten salts as well as variety of polyelectrolytes and colloidal suspensions. Equally well known are biological systems of proteins. All these systems are examples of soft matter strongly influenced, if not dominated, by long-range forces. For more than half of century the classical theories by Debye and Hückel as well as by Derjaguin, Landau, Verwey and Owerbeek (DLVO) have been at the basis of theoretical physical chemistry and chemical engineering. The substantial progress in material science during last few decades as well as the advent of new instrumentation and computational techniques made it apparent that in many cases the classical theories break down. New types of interactions (e.g. hydrodynamic, entropic) have been discovered and a number of questions have arisen from theoretical and experimental studies. Many of these questions still do not have definite answers.

Molecular Thermodynamics of Nonideal Fluids serves as an introductory presentation for engineers to the concepts and principles behind and the advances in molecular thermodynamics of nonideal fluids. The book covers related topics such as the laws of thermodynamics; entropy; its ensembles; the different properties of the ideal gas; and the structure of liquids. Also covered in the book are topics such as integral equation theories; theories for polar fluids; solution thermodynamics; and molecular dynamics. The text is

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recommended for engineers who would like to be familiarized with the concepts of molecular thermodynamics in their field, as well as physicists who would like to teach engineers the importance of molecular thermodynamics in the field of engineering.

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