Norikazu OHTORI, Dr. Sci.

Professor
Program: Fundamental Sciences
Area: Chemistry
Undergraduate: Dept. of Chemistry

Professional Expertise

He specializes in physical chemistry and studies microscopic structure and transport properties of liquids and glasses from the viewpoint of statistical mechanics. His career started with experimental works using spectroscopic and diffraction methods on molten salts about 33 years ago. Initially, molecular simulation was used as a complementary method to them, but now it has become a main research method. Molecular simulation has become a very powerful tool in material sciences since the efficient method of the first principles calculation based on quantum mechanics developed by Car and Parrinello[1] and many researchers has become to use it. However, it still remains a heavy load on the present most computers to perform the calculations of time dependent properties of systems containing more than hundred atoms. Therefore, it would be very useful if they could consolidate information on the interatomic forces obtained from the first principles calculation as analytical functions, because they could perform the simulation with both efficiency in classical method and accuracy in quantum mechanical method. He now collaborates with Prof. Madden at University of Oxford and Prof. Salanne at UPMC, University of Paris 06, in order to perform such a realistic simulation mainly in ionic systems.

[1] R. Car and M. Parrinello, *Phys. Rev. Lett.*, 55, 2471 (1985).

Research Fields of Interest

He is interested in both structure and transport properties mainly of liquids, especially molten salts. He also studies aqueous solutions of alcohol, molecular liquids, and oxide glasses. Particularly, molten salts are useful as heat media in high-temperature energy conversion systems, because they are stable both at high temperatures and for wide temperature ranges. He has successfully applied the simulation method to the evaluation of the thermal conductivity of many ionic systems including molten salts at high temperatures, because the experimental evaluations are very difficult for them, and established an empirical law working well in these systems.

Education

1990: Doctorate of Science in Chemistry, Graduate School of Science and Technology, Tokyo Institute of Technology, Japan
1987: M.S. in Chemistry, Graduate School of Science, Nagoya University, Japan
1985: B.S. in Chemistry, Faculty of Science, Nagoya University, Japan

Professional Societies and Activities

1. The Chemical Society of Japan
2. The Electrochemical Society of Japan
3. The Molecular Simulation Society of Japan

Awards

1. Molten Salt Prize, 2011, Molten Salt Committee of the Electrochemical Society of Japan

Major Publications

Papers

[1] ”The Stokes-Einstein Relation for Non-spherical Molecular liquids”, *Chem. Lett.*, **49**, 379(2020).

[2] ”The Stokes-Einstein relation for simple fluids: From hard-sphere to Lennard-Jones via WCA potentials”, J. Chem. Phys., 149, 214501(7pp)(2018).

[3] “Breakdown of the Stokes-Einstein Relation in Pure Lennard-Jones Fluids: from Gas to Liquid via Supercritical States”, *Phys. Rev. E*, **94**, 012111(5pp)(2017).

[4] “Thermal Design Investigation for a Flinabe Blanket System”,
Fusion Sci. Technol., 72, 382-388(2017).

[5] “A DFT-Based Aspherical Ion Model for Sodium Aluminosilicate Glasses and Melts”, *J. Phys. Chem. C*, **118**, 3385-3391(2016).

[6] “Revisiting the Benford law: When the Benford-like distribution of leading digits in sets of numerical data is expectable?”, *Physica A*, **461**, 595-601(2016).

[7] “Molecular insights into the boundary conditions in the Stokes-Einstein relation”, *Phys. Rev. E*, **93**, 050104(R) (5pp) (2016).

[8] “Dynamic Behavior of Mesoscopic Concentration Fluctuations in an Aqueous Solution of 1-Propanol by MD Simulation”, *Chem. Lett.*, **45**, 98-100(2016).

[9] “Explicit expressions of self-diffusion coefficient, shear viscosity, and the Stokes-Einstein relation for binary mixtures of Lennard-Jones liquids”, *J. Chem. Phys.*, **143**, 164514(2015).

[10] “Evaluation of Physical Properties of the Molten Salt Mixtures Flinabe for a Fusion Blanket System Using Molecular Dynamics Simulation”, *Fusion Sci. Tech.*, **68,** 669-673(2015).

[11] “Transport coefficients and the Stokes-Einstein relation in molten alkali halides with polarizable ion model”, *Mol. Phys.*, **113**, 2442(2015).

[12] “DFT-based polarizable force field for TiO_2 and SiO_2”, *Modelling and Simul. Mater. Sci. Eng.*, **23**, 074005 (2015).

[13] “Explicit expression for the Stokes-Einstein relation for pure Lennard-Jones liquids”, *Phys. Rev. E*, **91**, 012111(7pp) (2015).

[14] “MD Study on the Thermal Conductivity of Molten Alkali Halides: Effect of Ionic Mass Difference”, *Int. J. Thermophys.*, **35**, 320-326(2014).

[15] “Thermal conductivity of simple liquids: Origin of temperature and packing-fraction dependences”, *J. Chem. Phys.*, **140**, 114502 (4pp) (2014).

[16] “Thermal Conductivity of Molten Alkali Metal Fluorides (LiF, NaF, KF) and Their Mixtures”, *J. Phys. Chem. B*, **118**, 3385-3391(2014).

[17] “Thermal conductivity of simple liquids: temperature and packing-fraction dependence”, *Phys. Rev. E*, **89**, 022129 (5pp) (2014).

[18] “Dynamic Structure Factor of Charge Density in Molten LiI by MD Simulation”, *Electrochemistry*, **82**, 152-155(2014).

[19] “Thermal Conductivity in Molten Alkali Halides: Composition Dependence in Mixtures of (Na-K)Cl”, *Mol. Simul.*, **38**, 432-436(2012).

[20] “Thermal Conductivity of Ionic Systems from Equilibrium Molecular Dynamics”, *J. Phys.: Condens. Matter*, **23**, 102101 (5pp) (2011).

[21] “Measurement of Wave Velocity Distribution in a Trabecula by Micro-Brillouin Scattering Technique”, *Jpn. J. Appl. Phys.*, **49**, 07HB05 (4pp) (2010).

[22] “Local Structure Analyses of Molten Lanthanum Trichloride – Alkali Chloride Ternary Systems: Approaches from Fundamentals to Pyrochemical Reprocessing”, *Electrochemistry*, **77**, 736-740(2009).

[23] “Calculations of the Thermal Conductivities of Ionic Materials by Simulation with Polarizable Interaction Potentials”, *J. Chem. Phys.*, **130**, 104507 (13pp) (2009).

[24] “Thermal Conductivity of Molten Alkali Halides: Temperature and Density Dependence”, *J. Chem. Phys.*, **130**, 044505 (5pp) (2009).

[25] “Observation of Induced Shear Acoustic Phonon by Brillouin Scattering”, *Jpn. J. Appl. Phys.*, **46**, (7B), 4626-4628(2007).

[26] “Local Structure of Molten $LaCl_3$ Analyzed by X-ray Diffraction and La-L_{III} Absorption- edge XAFS Technique”, *J. Alloys Compd.*, **408-41**, 248-252(2006).

[27] “Application of Brillouin Scattering to the Local Anisotropy and Birefringence Measurements of Thin Layers”, *Ultrasonics*, **44**, e1555- e1559 (2006):

[28] “XAFS Study of Barium Aluminoborate Glasses”, *Phys. Chem. Glasses*, **47**, 521-523(2006).

[29] “XAFS Study of Barium Borate Glasses and Crystals”, *Phys. Chem. Glasses*, **47**, 445-447(2006).

[30] “MD Study of Sodium Borate Glasses containing Al_2O_3”, *Phys. Chem. Glasses*, **47**, 323-327(2006).

[31] “Raman Spectroscopic Study of Ionic Association in Molten $LaCl_3$ and Molten CsCl-NaCl Mixtures”, *Electrochemistry*, **73**, 936-938(2005).

[32] “*In Situ* Raman Spectroscopic Observation of Corrosion Reaction of Fe with Na_2O_2 up to 833 K”, Electrochemistry, **73**, 675-679(2005).

[33] “Raman Spectra of Peroxide Ions at High Temperature”, *Electrochemistry*, **73**, 597-599(2005).

[34] “High Temperature La-LIII XAFS Analysis of $LaCl_3$ and LaOCl”, *Electrochemistry*, **73**, 710-714(2005).

[35] “MD Simulation of Molten (NaCl-2CsCl) Containing UO_2^{2+} with Fixed Intraionic Charge Distribution”,
Electrochemistry, **73**, 748-750(2005).

Book Chapters

[1] M. Salanne, C. Simon, P. Turq, N. Ohtori, P.A. Madden, 2013, *Molten Salts Chemistry From Lab to Applications*, Elsevier, pp.1-16.