International Workshop
Solution Chemistry; From Solvation to Biomolecules

Program

9:45~9:50

Opening Remarks. M. Terazima (Kyoto University)

Chair K. Ibuki (Doshisha University)

9:50~10:15

L1: Water-Alcohol Mixtures: What Have We Learnt from Molecular Simulation
I. Nezbeda (Charles University)

10:15~10:35

S1: Diffusion of Hydrophobic and Hydrophilic Molecules in Water and Organic Solvents. How are Solvations Reflected in Diffusion?
T. Tominaga (Okayama University of Science)

10:35~11:00

L2: Local Structure in Supercritical Ionic Solutions as seen by MD Simulations and EXAFS Spectroscopy
J.-C. Soetens (Universite Bordeaux 1)

Chair P. Bopp (Universite Bordeaux 1)

11:00~11:20

S2: Dynamics of Liquids with Strong Coulombic Interaction
T. Yamaguchi (Nagoya University)

11:20~11:45

L3: Modeling of Supramolecular Structure and Permittivity of Liquids in Quasichemical Approach: Methanol from Melting Point to Critical State
V. A. Durov (Lomonosov Moscow State University)

11:45~12:05

S3: Effect of the Solutes (Urea and Acetone) on the Structure of Water: A Molecular Dynamics Simulation
A. Idrissi (Laboratoire de Spectrochimie Infrarouge et Raman)

12:05~13:00

Lunch

Chair H. Sato (Kyoto University)

13:00~13:25

L4: The Raman Noncoincidence Effect of the S=O Stretching Mode of Neat Liquid Dimethyl Sulfoxide

M. Musso (University of Salzburge)

13:25~13:45

S4: Time-Domain Theoretical Analysis of the IR, Polarized Raman, and 2D-IR Spectra of Peptide Chains in Aqueous Solution

H. Torii (Shizuoka University)

13:45~14:10

L5: Association and Clusterization Phenomena in Electrolyte Solutions: Statistical Mechanical Modeling

M. F. Holovko (Ukraine Institute for Condensed Matter Physics)

14:10~14:30

S5: Ultrafast Vibrational Dynamics of Small Ions in Solution Studied by Nonlinear Infrared Spectroscopy

K. Ohta (Kobe University)

14:30~15:00

Coffee Break

Chair M. Terazima (Kyoto University)

15:00~15:25

L6: On Microscopic Interpretation of Volumetric Data

T. V. Chalikian (University of Toronto)

15:25~15:45

S6: Molecular Recognition Realized by the 3D-RISM Theory

F. Hirata (Institute for Molecular Science)

15:45~16:05

S7: FTIR Spectroscopic Imaging Applied to Atherosclerotic Aorta

F. Palombo (Imperial College London)

16:05~16:25

S8: Application of the 3D-RISM Theory of Molecular Solvation to Protein Aquesous Solution Systems

T. Imai (Ritsumeikan University)

16:25~16:55

Coffee Break

Chair Y. Kimura (Kyoto University)

16:55~17:15

S9: Structure and Dynamics of Moelcules and Ions in Room Temperature Ionic Liquids

C. Wakai-Furutani (Kyoto University)

17:15~17:35

S10: Cesium Formate: A Computational Study

P. Panchmatia (Uppsala Univesitet)

17:35~17:55

S11: $Au(CN)_2^+$ and its Solvation in Nitromethane

M. Probst (Innsbruck University)

17:55~18:00

Concluding Remarks. Y. Kimura (Kyoto University)