Satellite Meeting of ICMS2013 in Sendai

"Molecular Simulation of Liquids and Interfaces"



Organizer The Molecular Simulation Society of Japan

Theoretical and Computational Chemistry Initiative

Date November 22 (Fri.), 2013

Place Lecture Room 4, Department of Chemistry

Tohoku University

(東北大学化学系講義棟 第四講義室)

Program

13:00 - 14:00 Ward H. Thompson (University of Kansas)

Dynamics of Nanoconfined and Bulk Liquids

14:00 - 14:30 Shinji Kajimoto (Tohoku University)

Hydrogen-Bond Breaking during Phase Separation in Triethylamine-Water Mixture: A Molecular Dynamics Study

14:45 - 15:45 Pavel Jungwirth (Academy of Sciences of the Czech Republic)

Photoionization in Water: Electrons, Cationic Holes, and DNA Damage

15:45 - 16:15 Tatsuya Ishiyama (Tohoku University)

Structure and Vibrational Spectra at Water/Vapor and Ice/Vapor Interfaces: Molecular Dynamics Study Combined with QM/MM Calculations

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