

## Theoretical Symposium "Frontiers of Quantum Chemistry"

Kwansei Gakuin Kaikan, Kwansei Gakuin University, Nishinomiya  
<http://www.kwansei.ac.jp/index.html>

November 11, 2015

10:00-11:00 **Keiji Morokuma (Kyoto University)** "Fascinating World of Theoretical Studies of Chemical Reactions: From Gas Phase Reactions to Organic Reactions, Catalysts, and Enzymatic Reactions"

11:00-12:00 **Hiroshi Nakatsuji (Quantum Chemistry Research Institute;QCRI)**  
"Chemistry of the Excited States of Molecules Studied by the SAC-CI Theoretical Methodology"

12:00-13:00 Lunch

13:00-13:50 **Kaoru Yamanouchi (University of Tokyo)** "Ultrafast molecular imaging by Coulomb explosion and laser assisted elastic electron scattering"

13:50-14:40 **Satoshi Yabushita (Keio University)** "Theoretical Studies of the Intensities for XH (X=C,O) Stretching Vibrations"

14:40-15:00 Break

15:00-15:50 **Masahiro Ehara (Institute of Molecular Science)** "Recent Developments and Applications of SAC-CI"

15:50-16:40 **Marek J. Wojcik (Jagiellonian University)** "Vibrational Spectroscopy of Hydrogen-Bonded Complexes, Liquids and Solids"

16:40-17:20 **Yukihiro Ozaki (Kwansei Gakuin University)** "Quantum Mechanical Interpretation of Intermolecular Vibrational Modes of Crystalline Polymers Observed in Low-Frequency Raman and Terahertz Spectra"

17:30-19:30 Reception

Kwansei Gakuin University School of Science and Technology    Ozaki Lab