

# Hajime TORII



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**【Specialty】** Theoretical chemistry

**【Keywords】** Vibrational spectroscopy, Intermolecular interactions, Liquids, Peptides

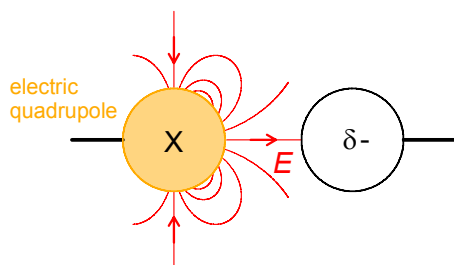
## 【Research Subject】

Theories of analysis for better understanding on the changes in vibrational band intensities and shapes induced by intermolecular interactions

## Research Group Activity

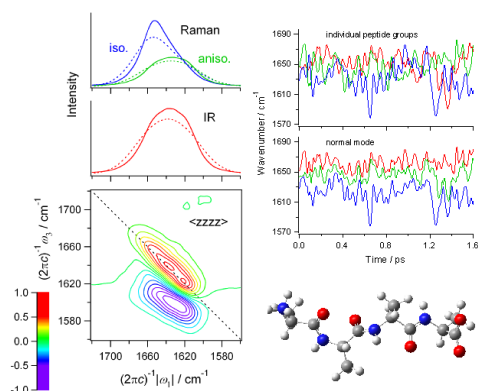
- Physicochemical Picture of Halogen Bonding

The electronic structural properties and the effects on vibrational spectra



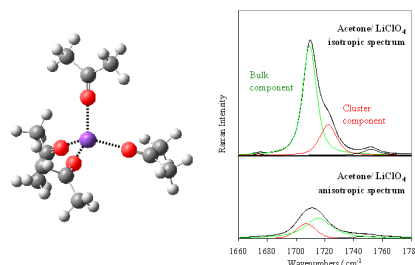
- Vibrational Band Profiles of Hydrated Peptide Chains

Calculations and analysis of 1D and 2D vibrational spectra using time-domain method



- Liquid Structures around Metal Ions and Vibrational Spectra

Characteristics of polarized Raman spectra and liquids structures



- Vibrational Band Profiles due to Weakly Resonant Vibrational Coupling
- Merger and intensity bias arising from vibrational coupling between different species

