Frontier Chemistry Center
フロンティア化学教育研究センター 講演会

演 題：**Spectroscopy of hydrogen bond - theoretical modeling of spectra and proton tunneling**

講 師：**Prof. Marek J. Wójcik**

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日 時：2013 年 4 月 17 日（水）13:00～14:00

場 所：理学部 7 号館 2 階 7-2-19 室

要 旨：I will discuss theoretical model for vibrational spectra of hydrogen-bonded systems which considers adiabatic coupling between high and low-frequency modes in hydrogen bonds, linear and quadratic distortions of the potential energy for the low-frequency vibration in the excited state of the high-frequency vibration, resonance interactions between hydrogen bonds, Fermi resonance, and mechanical and electrical anharmonicities. Comparison between experimental and theoretical spectra will be presented for different hydrogen-bonded systems. Results of Car-Parrinello molecular dynamics used to calculate infrared spectra of crystalline imidazole will be also presented. Proton tunneling in tropolone will be described by two-dimensional model potentials fitted to quantum-mechanicaly calculated grids of energies, and used to reproduce experimental promotion of the tunneling by the excitation of the planar modes and suppression by excitation of the out-of-plane modes.

本講演は『化学研究先端講義／総合化学特別研究第二』の一部として認定されています

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