第 688 回　化学･物質工学セミナー開催のお知らせ

下記の通り、化学･物質工学セミナーを、工学研究科 5 年一貫制博士課程グリーンシステム創成科学専攻の国際セミナーと共催します。万障お繰り合わせの上、ご参加下さい。

Vibrational Spectroscopy of Hydrogen-Bonded Complexes, Liquids and Solids

Marek J. Wójcik

Faculty of Chemistry, Jagiellonian University, Poland

記

日時:　平成 30 年 1 月 12 日（金） 16:40 ~ 18:10

場所:　長崎大学文教キャンパス　サイエンス＆テクノラボ 2 階　セミナー室 2

Abstract

Theoretical model is presented for the X-H(D) stretching vibrations in hydrogen-bonded systems. The model takes into account adiabatic coupling between the high-frequency X-H(D) stretching and the low-frequency intermolecular X...Y stretching modes, linear and quadratic distortions of the potential energy for low-frequency vibrations in the excited state of X-H(D) stretching vibration, resonance interactions between hydrogen bonds, Fermi resonance between X-H(D) stretching and the overtone of X-H(D) bending vibrations, and mechanical and electrical anharmonicities. The effects of deuteration and temperature on spectra are successfully reproduced by the model. Comparison between experimental and theoretical spectra is presented for different hydrogen-bonded systems, including ice. We present also the method of Car-Parrinello molecular dynamics used to calculate infrared spectra of crystals.

Proton tunneling in tropolone is described by two-dimensional model potentials. The potentials have been fitted to quantum-mechanically calculated two-dimensional grid of energies, and used to analyze proton dynamics. The model PES well reproduces experimentally observed promotion of the tunneling by the excitation of the planar modes and suppression by the excitation of the out-of-plane modes.

是非、多数の皆様のご参加をお待ちしております。

本セミナーオーガナイザー

長崎大学大学院工学研究科　相樂 隆正 及び Bun Chan

Tel: 095-819-2676 (相樂)　095-819-2647 (B. Chan)

問い合わせ E-mail: sagara@nagasaki-u.ac.jp (相樂)

以　　上