グローバル COE 物質科学イノベーション講演会

演 題：**Theoretical Modeling of Vibrational Spectra and Multidimensional Proton Tunneling in Hydrogen-Bonded Systems**

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要 旨：Theoretical model is presented for the X-H(D) stretching vibrations in hydrogen-bonded systems. The model takes into account an adiabatic coupling between the high-frequency X-H(D) stretching and the low-frequency intermolecular X...Y stretching modes, resonance interactions between two equivalent hydrogen bonds in the dimer, Fermi resonance between the X-H(D) stretching and the overtone of the X-H(D) bending vibrations, and mechanical and electrical anharmonicities. The model successfully reproduces the effect of deuteration. Comparison between experimental and theoretical spectra is presented for hydrogen- bonded crystals and their deuterated analogues.

Multidimensional proton tunneling in symmetric hydrogen-bonded systems is described by two-dimensional model potentials. The potentials have been fitted to quantum-mechanicaly calculated two-dimensional grid of energies, and used to analyze proton dynamics in tropolone. The model PES quantitatively reproduce experimentally observed promotion of the tunneling by the excitation of the planar modes and suppression by the 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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