

Nonlinear vibrational spectroscopy of aqueous systems: Use of spectral maps and beyond



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Currently at: CLS, Institute of Integrated Research, Institute of Science Tokyo

Time & Date: 13:30-15:30, Thursday 08 May 2025

Place: The 3rd Seminar Room, R1 bldg. Suzukakedai campus
(R1棟2F 第三会議室)

Abstract: We will present our recent theoretical work on nonlinear vibrational spectroscopy of aqueous systems using a combination of molecular dynamics simulations, quantum calculations and machine learning methods. Specifically, we will present calculations of one-dimensional and two-dimensional vibrational sum frequency generation (1D-VSFG and 2D-VSFG) and 2D-IR spectroscopy of aqueous surfaces and bulk systems, including acidic and basic solutions. The results of various dynamical features of the two-dimensional spectra will be connected to various underlying dynamical modes of the systems involving hydrogen bonded motion and proton transfer processes in case of acidic and basic solutions.

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