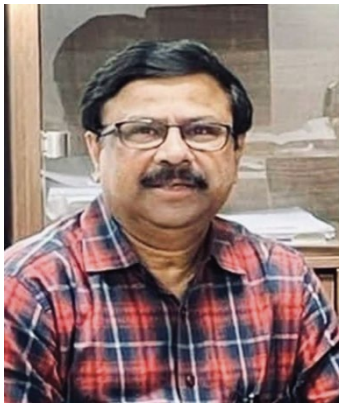
第489回触媒科学研究所コロキウム

Proton Transfer Dynamics in Aqueous Acidic and Basic Solutions and Nonlinear Vibrational Spectroscopy from Ab Initio Molecular Dynamics



Prof. Amalendu CHANDRA
(The Indian Institutes of Technology Kanpur)

2025年8月8日(金) 15:00–16:00

創成科学研究棟 5階 大会議室

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We will discuss our recent theoretical work on proton transfer and nonlinear vibrational spectroscopy of aqueous solutions of strong acids and bases. Our study is based on ab initio molecular dynamics simulations and time correlation function approaches of nonlinear vibrational spectroscopy. We will present calculations of the rate constants of proton transfer including proton rattling and proton translocation, and connect them to the observables of two dimensional infrared spectroscopy

Amalendu Chandra is a Professor in the Department of Chemistry and also currently a Specially Appointed Professor at the Institute of Science Tokyo. Earlier, he was Dean of Research and also Dean of Faculty Affairs at IIT Kanpur. He obtained his PhD in 1991 from Indian Institute of Science Bangalore. Subsequently, he worked as a Postdoctoral Fellow at the University of British Columbia for two years before joining IIT Kanpur as an Assistant Professor in 1993. He is a Fellow of all Science Academies of India. He also received Alexander von Humboldt Fellowship from Germany and JSPS Invitational Fellowship from Japan. He works broadly in the area of theoretical studies of structure, dynamics, and spectroscopy of liquids, interfaces, confined systems, clusters, and also chemical reactions in biological systems.

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489th Institute for Catalysis (ICAT) Colloquium