## Theory of Surface Nonlinear Spectroscopy

## Overview

Sum Frequency Generation (SFG) spectroscopy is a powerful optical probe method of interfaces with excellent selectivity and sensitivity. Now it is widely used to interfaces in various disciplines, including electrochemistry, biophysics, polymer science, heterogeneous atmospheric chemistry, biological membranes, etc. It can provide rich microscopic information on various interfacial structures, however we often encounter difficulties in interpreting the observed spectra when we use the spectroscopic tools. The main difficulty to use this powerful technique lies in the interpretation, and thus solid theoretical background is desirable. This course offers a unified and comprehensive theory of SFG spectroscopy. The theory is based on fundamental quantum mechanics and electromagnetics, which are also relevant to the theoretical background of general spectroscopy.

The present course is designed to provide the fundamentals of the SFG spectroscopy and its importance towards surface and interface science. At the end of the course, the participants are expected to get a deeper understanding about the following topics: Electrodynamics at Interface, Response to incident lights, boundary conditions at the interface, summary of factors in SFG spectra, Quantum mechanical theory of nonlinear polarization, density matrix, perturbation form of second order nonlinear susceptibility, vibrational resonance, relation to molecular orientation, molecular theory of local field. The course would also cover the computational schemes of SFG: energy and time-dependent representations.

The main objectives of this course are to achieve the followings:

i) Exposing participants to the fundamentals of quantum and electromagnetic theories related to spectroscopy

- ii) Providing firm background theory of the SFG spectroscopy
- iii) Familiarizing participants to the theoretical analysis of interfaces and spectra

iii) Providing exposure to basic problems and solutions of the spectroscopy

Modules	Theory of Surface Nonlinear Spectroscopy, September 26-30, 2022
You Should Attend If	<ul> <li>you are an engineer, or research scientist working in the field of 'Nonlinear Laser Spectroscopy' at the surface and interface.</li> <li>You are performing computational work on sum frequency generation spectroscopy to probe interfaces and surfaces.</li> <li>you are a student (MTech/MSc/PhD) or faculty from academic institutions interested in learning the fundamental of quantum mechanics and electromagnetics towards the formulations of sum frequency generation spectroscopy which is a second order nonlinear optical process.</li> </ul>
Fees	The participation fees for taking the course is as follows: Academic Institutions: Rs 4000 (Faculty) and Rs 2000 (Student) Industry / Research Organizations: Rs 8000 Participants from abroad: US \$250 The above fee includes all instructional materials, computer use for tutorials and assignments, Lodging and Boarding are NOT included in the fees. The participants will be provided with accommodation on payment basis (subject to the availability in the hostels/guest house at IIT Ropar)

## The Faculty



**Prof. Akihiro Morita** was born in Kamakura, Japan, in 1964. He received his Bachelor's and Master's degrees in science from the University of Tokyo, and a Ph. D. in chemistry from Kyoto University in 1995. He was a research associate at Kyoto University and then an associate professor at the Institute for Molecular Science before moving to Tohoku. He also worked as a research associate at the University of Colorado from 1999 to 2000 with Prof. Casey Hynes. He is currently a professor in chemistry at Tohoku University since 2007. His research interests are centered

on electronic structure and molecular dynamics in solutions and their interfaces. He is particularly interested in liquid interfaces and related phenomena, including nonlinear spectroscopy, mass transport, and heterogeneous reactions.



**Dr. Kailash Chandra Jena** is an associate professor at the Indian Institute of Technology, Ropar. He received his Ph.D. degree in 2008 from the Indian Institute of Technology, Madras. His current research interest is sum-frequency generation (SFG) vibrational spectroscopy and its application to probe the molecular structure of various molecules and their interactions with interfacial water molecules at air/water. His research priorities are mainly focused on protein-protein interaction, nanomaterial for sensing application, drug-polymer interaction, specific ion effects,

evaporation process, self-assembly of molecules, and laser-induced microjet formation.

## Course Co-ordinator

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