

CH-621

Theory of nonlinear electronic and electronic-vibrational spectroscopies

Yoshitaka Tanimura

Cursus	Sem.	Type
Chimie et génie chimique		Obl.

Language	English
Credits	1
Session	
Exam	Term paper
Workload	30h
Hours	16
Lecture	12
Practical work	4
Number of positions	

Frequency

Only this year

Remarque

Fall 2019

Summary

In this course, Prof Tanimura will teach the theoretical basis of multidimensional electronic and electronic-vibrational spectroscopies. The methodology will be illustrated by calculating multidimensional signals using optical Liouville pathways and reduced equations of motion.

Content

Theory of nonlinear electronic and electronic-vibrational spectroscopies

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Spectral line shapes in the condensed phase contain information on various dynamic processes that modulate the transition energy, such as microscopic dynamics, inter- and intramolecular couplings, and solvent dynamics. In this course, I will teach the theoretical basis of multidimensional electronic spectroscopies (2DES) and 2D electronic-vibrational spectroscopies (2DEVS). I will explore and describe the roles of different physical phenomena that arise from the peculiarities of dissipative dynamics in multidimensional spectra. The methodology will be illustrated by calculating multidimensional signals using optical Liouville path and reduced equations of motion approaches. A Brownian oscillator model with the nonlinear system-bath interaction will be employed to explain how fluctuation and dissipation arises from the environment. Using the hierarchy formalism, one can precisely calculate multidimensional electronic spectra for a multistate anharmonic system. The distributed source code, "nonMarkovian2009+2DES" will be demonstrated and examined.

REFERENCES:

- [1] Y. Tanimura, J. Phys. Soc. Jpn, 75, 082001 (2006).
- [2] Y. Tanimura, J. Chem. Phys 137, 22A550 (2012).
- [3] T. Ikeda and Y. Tanimura, J. Chem. Phys. 146, 014102 (2017).
- [4] T. Ikeda and Y. Tanimura, Chem. Phys. 515, 203 (2018).
- [5] T. Ikeda and Y. Tanimura, J. Chem.Theo. Comp.15 2517 (2019).

CONTENTS

1. Introduction
2. Observables in multidimensional spectroscopies
3. Optical Liouville paths and Albrecht diagrams
4. Response function approach
5. Reduced equation of motion approach.
6. Hierarchical Equation of Motion approach

Keywords

multidimensional electronic spectroscopies, 2D electronic-vibrational spectroscopies, response function theory

Resources**Bibliography****REFERENCES:**

- [1] Y. Tanimura, J. Phys. Soc. Jpn, 75, 082001 (2006).
- [2] Y. Tanimura, J. Chem, Phys 137, 22A550 (2012).
- [3] T. Ikeda and Y. Tanimura, J. Chem. Phys. 146, 014102 (2017).
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Websites

- <http://theochem.kuchem.kyoto-u.ac.jp/members/tanimura.htm>