Title of the course:

Polarizability relaxation: From archetypal molecular liquids to deep eutectic solvents

SYLLABUS

1 Lecturer information

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2 Title of the course

Polarizability Dynamics in Liquids. Principles and Applications.

3 Course program

This course contents include: *i* – an overall presentation of the Raman and infrared vibrational spectroscopies and the corresponding discussions covering briefly and semi-qualitatively the theoretical foundations underlying the scope of the course: namely the Wiener-Khinchin theorem and the fluctuation-dissipation theorem. *ii* – a review of a few representative cases in the literature that deal with the dynamical analysis of far infrared and low-frequency Raman spectroscopy from both theoretical and experimental approaches. *iii* - a few practical spectroscopic approaches to achieve dynamical information of a variety of classical archetypal liquids as well as the emerging materials such as ionic liquids and deep eutectic solvents. iv – the use of molecular dynamics, MD, simulations as an important tool to unveil dynamical information valuable for spectroscopic analysis. In summary, this course intends to provide students with an overall view of both theoretical and experimental approaches dealing with low-frequency vibrational spectroscopies as tools for achieving dynamical information about liquids.

4 Course content detailed per lesson of two hours

Lesson 1 – Deep eutectic solvents, DESs - I - principles and applications. Throughout this lesson, students will be presented with introductory concepts, a brief relevant history, the usual classification system, required characterization techniques, and a few electrochemical applications of deep eutectic solvents, DESs.

Lesson 2 – Deep eutectic solvents, DESs – II - molecular dynamics and vibrational spectroscopy. Following the introduction to DESs provided in Lesson 1, the subject will be further explored using theoretical tools (molecular dynamics simulations) and vibrational spectroscopy. After a brief introduction to the models and techniques, students will examine a selection of articles chosen both for their didactic features and scientific relevance.

Lesson 3 – MD and low-frequency vibrational spectroscopy of archetypal molecular liquids. In this lesson, molecular dynamics (MD) simulations will be explored from their basic principles to provide theoretical data comparable to low-frequency optical spectra of archetypal liquids. Emphasis will be given to the use of such theoretical data to: i – validate the theoretical results achieved and ii – provide a complementary understanding of the corresponding experimental data.

Lesson 4 – Molecular dynamics, MD, simulation of ionic liquids, ILs. After a lesson devoted to archetypal molecular liquids, the focus of this lesson is on liquid systems comprised of charged particles. This lesson will reinforce the concepts and discussions of the previous lessons in the context of ILs.

Lesson 5 – Protic ionic liquids, pILs: MD and low-frequency spectroscopy. Along this section, the main subject will be revisited and applied to an alternative context. This lesson will offer students a fair discussion on how the combination of strong non-directional Coulombic interactions and hydrogen bonds impacts spectroscopic properties.

Lesson 6 – Formic acid: a test case. In this lecture, students will be able to conduct short molecular dynamics simulations, execute introductory model evaluations, and produce early data related to polarizability relaxation.

5 Suggested reading

As a suggested reading basic literature available on Raman spectroscopy and molecular dynamics simulation.

6 Learning Objectives

The main objective of the present course is to provide students with the basic theoretical foundations required for the proper analysis of low-frequency vibrational spectra of archetypal liquids. The overall discussions are complemented in order to encompass emerging materials such as ionic liquids and deep eutectic solvents, couplet with experimental bases discussions of real system. The main goal is to unveil theoretical framework underlying vibrational spectroscopy as a source of dynamical information in liquids.

7 Knowledge and Skills to be acquired

This course will provide students with a theoretical background carefully chosen and adapted for a general audience, which will serve as the formal basis for the main concepts used throughout the course. This course will also provide students with basic tools to perform simple calculations

comparable with corresponding experimental data. This course will provide students with the necessary foundations to critically interpret low-frequency vibrational spectroscopy results, thereby increasing the chances of using these tools for conduct research projects.

8 Prerequisites

Graduation in Chemistry, Physics or equivalent is recomended for the general purposes of this course.

9 Teaching Methods

- MODE 1 - Pre-recorded lessons uploaded on the moodle platform (a meeting must be organized with PhD students in order to clarify eventual doubts)

- MODE 2 (preferred) - Lessons delivered in-person and in remote with simultaneous recording by the WEBEX platform

(The lessons must be recorded and available to all the students that cannot take part to the lessons in streaming. The Webex platform must be used. All course content should be uploaded to the Moodle platform on the Chemical Sciences PhD page "Courses and Seminars of the PhD in Chemical Sciences 2022-2023")

10 Further information

Students will be evaluated based on attendance and the submission of a series of **"One-Minute Papers"** at the end of each lecture. These brief reflections require students to summarize the core scientific concept learned and identify a remaining research question, ensuring continuous engagement and critical thinking throughout the six-lecture series.

11 Type of Assessment

The student can choose one of the following options.

1. Discussion of the most important aspects of the studied topics.

2. A short written text in a free format that summarizes the lectures' contents.

3. Discussion of an assigned article.

12 Period

4 June - 2h - Deep eutectic solvents, DESs - 1 - principles and aplications.
5 June - 2h - Deep eutectic solvents, DESs - 2 - Molecular Dynamics and vibrational spectroscopy.
9 June - 2h - Molecular Dynamics and vibrational spectroscopy of archetypal molecular liquids.
11 June - 2h - Molecular Dynamics simulation of ionic liquids, ILs.
16 June - 2h - Protic Ionic Liquids, pILs: Molecular Dynamics.
18 June - 2h - Protic Ionic Liquids, pILs: Raman spectroscopy and evaluation.