PRIN 22 Project – SPIRAL - Lossless surface waves for chiral spectroscopy
Intermediate Project Meeting
SAPIENZA Università di Roma - Dipartimento di Scienze di Base e Applicate per l' Ingegneria
Oct 30th -31st 2024

PROGRAM OF THE MEETING

Wednesday October 30th (welcome to SPIRAL partners) – Building RM009 – Sala Lettura

12:00-14:00 **Welcome and lunch** (only SPIRAL partners)

Wednesday October 30th (Open Workshop) – Building RM004 – Aula Seminari

14:00-14:15 **Introduction** *Francesco Michelotti*, SAPIENZA Università di Roma
Paolo Biagioni, *SPIRAL Project PI*, Politecnico di Milano

14:15-15:00 **Tutorial #1** Surface electromagnetic waves on truncated one-dimensional photonic crystals (1DPC)
Francesco Michelotti, SAPIENZA Università di Roma

Abstract

After a short historical introduction to surface electromagnetic waves (SEW) sustained by all dielectric layered structures (1DPC), the presentation will focus on their physical properties. In particular we shall review the impact of the design of the 1DPC on the quality factor of the resonances, on the propagation length and on the field localization at the 1DPC surface. Sensitivity and resolution of label-free SEW biosensors with respect to perturbations of the refractive index at the 1DPC surface will be discussed in detail. Coupling between an emitter placed in proximity of the 1DPC surface and the SEW is then discussed with particular emphasis on the emitter/1DPC distance and on the polarization. Applications of SEW in gas-sensing, bio-sensing, microscopy, integrated photonics, and nonlinear optics will also be reported.

15:00-15:45 **Tutorial #2** From Chirality to Superchirality, from Molecules to Light
Giovanni Pellegrini, Università Degli Studi di Pavia

Abstract

The geometrical property of three-dimensional objects that cannot be superimposed to their mirror image is called chirality. Identical objects with opposite chirality, known as enantiomers, share most chemical and physical properties, and display their chiral nature only in the interaction with a chiral environment. Chirality is fundamental in biological processes and is prevalent in biomolecules, with DNA being a prime example. Light itself exhibits chiral properties and can be used to probe the chirality of chemical compounds, though these interactions are typically very weak, making it challenging to analyze small amounts of molecules. In this seminar, we will first introduce the concept of optical chirality and then explore how plasmonic and photonic nanostructures can create superchiral fields, electromagnetic fields that interact strongly with small quantities of chiral molecules, enabling the detection of their chiral properties. Special focus will be given to superchiral surface waves, a unique type of electromagnetic field that potentially allows for the analysis and manipulation of chiral objects at the nanoscale.

15:45-16:15 **Coffee break**

16:15-17:00 **Tutorial #3** DFT calculations of molecular CD
Matteo Tommasini, Politecnico di Milano

Abstract

By measuring the interaction between light and matter, spectroscopy can reveal the molecular details of a sample's structure, such as its chirality. Spectroscopic observations are the direct manifestation of quantum transitions that occur in the sample stimulated by the light source used in the instrument. For this reason, the interpretation of experimental data is facilitated by the availability of accurate methods that allow for calculating quantum transitions, from which one can simulate spectra. Since its first appearance in chemistry in the '90s, Density Functional Theory has evolved into a practical computational technique by which molecular spectra can be simulated and efficiently interpreted. This applies to many vibrational and electronic spectroscopies, including circular dichroism (CD). This tutorial will compactly review the basic workflow for obtaining a simulated CD spectrum, starting from a given chiral molecular structure. The fundamental theoretical background will be discussed to illustrate the adopted computational framework and its application to representative examples.

17:00-17:45 **Tutorial #4** Synthesis of chiral molecules
Elisabetta Brenna, Politecnico di Milano

Abstract

The presentation will first introduce the basic concepts of molecular chirality (definition, criteria for identifying chiral molecules, distinction between enantiomers and diastereoisomers), then the possible strategies for the synthesis of the enantiomers of chiral compounds will be summarised. A special focus will be devoted to biocatalytic methods, discussing their advantages and disadvantages. The immobilisation of enzymes and their application in continuous flow reactors will also be briefly described.

Thursday October 31st (restricted to SPIRAL partners) – Building RM004 – Aula Seminari

09:00-09:30 The project and its objectives (Polimi)

09:30-10:00 Surface functionalization (Sapienza and Polimi)

10:00-10:30 Coffee break and visit of the laboratories at SAPIENZA and at IIT

10:30-11:00 Simulations for superchiral surface waves (UniPV)

11:00-11:30 DFT activity (Polimi)

11:30-12:30 Perspectives and next steps

12:30-13:30 Visit of the laboratories at SAPIENZA and at IIT

13:30-15:00 Lunch