Istituto per la Microelettronica e Microsistemi

Consiglio Nazionale delle Ricerche

AT3 Technological Area Modelling

WEBINAR: Modelling and Spectroscopy

MERCOLEDI' 13 DICEMBRE 10:00-12:00

https://meet.goto.com/604347029

ORE 10:00 *INTRODUCTION, Giuseppe Fisicaro* IMM CATANIA SEDE

ORE 10:05 *CHAIR Antonio Valletta* IMM ROMA

Alberto Debernardi (theory) and *Alessio Lamperti* (experiment) IMM AGRATE.

"X-ray absorption near edge structure (XANES) spectroscopy: an improved understanding by matching first principles and experiment"

Combining first principles and experimental spectroscopy is a powerful strategy to enlighten and identify microscopic processes in solids. Here, we apply such strategy to O K-edge XANES in $Zr_{1-x}Fe_xO_{2-y}$, a dilute magnetic oxide, with Fe from x~0.06 to x~0.25 % at., to find its structure and magnetic order at low and room temperature. Zr substitution by Fe atoms radically changes O XANES spectrum, especially due to pre-edge peak appearance, ascribed to O 1s to O 2p dipole transitions hybridized with unoccupied Fe 3d states, and seen to increase at increasing Fe concentration, suggesting the increase of unoccupied Fe 3d states. By comparing ab-initio and experimental data, we show that the effect of Fe atoms is localized in the first shells surrounding each Fe atom disappearing when moving far from them. The pre-edge peak increase with Fe amount relates to an increase of Fe atoms simultaneously associated to the decrease of the number of O atoms located in shells of order higher than 2.

ORE 10:30 *CHAIR Antonio Valletta* IMM ROMA

Fabio Della Sala (theory) IMM LECCE.

"Time-Dependent Density Functional Theory: from molecules to plasmonic nanoparticles"

I review the main equations of the Time-Dependent Density Functional Theory (TDDFT) for the calculation of absorption spectra of molecules and extended systems. Recent developments and approximations are discussed in terms of efficiency and accuracy. To model the optical properties of large nanosystems, such as metal nanoparticles, the orbital-free version of TDDFT, also known as the Quantum Hydrodynamic Theory(QHT), is introduced. Relations between classical electrodynamics, QHT and TDDFT are discussed in the context of plasmonic nanosystems.

Adriano Colombelli (theory&experiment) IMM LECCE.

"Numerical Modeling: Key to Advanced Plasmonic Metamaterials in Optical Sensing"

This work will focus on numerical modeling's crucial role in designing and optimizing plasmonic nanostructures for optical transducers in bio-chemical sensing. Emphasizing nanotechnology's intricate light-matter interplay, numerical simulations provide precise insights into plasmonic metamaterial physics, enabling the fabrication of tailored structures. The motivation stems from the crucial role numerical modeling plays in various applications, specifically in improving sensitivity in sensing. The study extends to plasmon-enhanced spectroscopies, optimizing metamaterials for advanced material analysis. Numerical simulation transcends design, streamlining the fabrication process, replacing trial-and-error strategy with virtual testing. This not only expedites optimization but drastically reduces time and cost, ensuring an efficient, cost-effective realization of plasmonic nanostructures. The dual emphasis on design and fabrication underscores numerical modeling's impact on advancing optical sensing applications.

ORE 10:55 *CHAIR Marco Pieruccini* IMM BOLOGNA

Ioannis Deretzis (theory) and *Salvatore Valastro* (experiment) IMM CATANIA.

"Temperature-Dependent Excitonic Band Gap in Bismuth Halide Single Crystals: Spectroscopic Ellipsometry and DFT calculations"

We study the optical behavior of bismuth-based low-dimensional perovskite single crystals ($Cs_3Bi_2Cl_9$, $Cs_3Bi_2Br_9$, $Cs_3Bi_2I_9$, and $MA_3Bi_2I_9$) by means of spectroscopic ellipsometry and density functional theory, coupled to the Bethe-Salpeter equation formalism. A strong excitonic peak is detected for all materials, arising from photogenerated electron-hole Coulomb interactions, whereas the threshold of continuous absorption is found at higher energies. The resonances of the excitonic and continuous bands along with exciton binding energies are extracted from a Critical Point Analysis of the ellipsometric data in a wide range of temperatures (–90 to 90°C), showing fine differences in the optical characteristics for each single crystal. Theoretical calculations allow for a critical assessment of the experimental data and correlate the optical properties with the distinct structure of each system.

ORE 11:20-12:00 *FREE DISCUSSION, QUESTIONS, PROPOSALS, CHAIR Marco Pieruccini* IMM BOLOGNA