



Seminar@ISM

organized by
Communications Group



CNR
Istituto di Struttura
della Materia

When?

May 05, 2025
3:00 PM (CEST)

Where?

@ Aula IB09
Area di Ricerca -
CNR Tor Vergata
Rome



Energy & Environment

05

May 2025

Maurizia Palummo

INFN, Department of Physics, University of
Rome "Tor Vergata"
Italy

Ab-initio Insights into the Opto-Electronic Properties of Emerging 2D and Layered Materials

The development of next-generation opto-electronic technologies relies on the discovery and understanding of novel low-dimensional materials. In this context, first-principles (ab-initio) simulations play a crucial role in unveiling the microscopic mechanisms that govern their properties, and in guiding experimental efforts through reliable predictions.

In this talk, I will present results obtained over the last years through parameter-free atomistic simulations aimed at exploring and tuning the opto-electronic properties of emerging 2D and layered materials. Using Density Functional Theory (DFT) and Many-Body Perturbation Theory (MBPT) approaches, such as GW and the Bethe-Salpeter Equation (BSE), we investigate: (i) electronic band gap renormalization, (ii) strong light-matter interaction, (iii) excitonic effects and radiative lifetimes, and (iv) the role of doping and chemical substitution as tuning mechanisms.

Particular attention will be devoted to materials families of interest for opto-electronic applications, including Transition Metal Dichalcogenides (TMDs) and 2D/layered halide perovskites. I will also discuss the excitonic properties of the MoSi_2N_4 family and carbon-based 2D triangulene polymers, highlighting their potential in emerging technologies.

Info at

www.ism.cnr.it/seminar-ism

comunicazione@ism.cnr.it

palummo@roma2.infn.it

