Institut Ruder Boskovic
ZAVOD ZA TEORIJSKU FIZIKU
Bijenicka c. 54
Zagreb, Hrvatska

SEMINAR ZAVODA ZA TEORIJSKU FIZIKU

Modelling interacting chromophores: aggregates and energy transfer

Mattia Anzola
University of Parma

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Abstract:

In molecular systems intermolecular forces are much weaker than the chemical bonds inside each individual molecular unit. I will present two examples of system where weak intermolecular interactions can markedly affect optical properties. In molecular aggregates, optical spectra cannot be calculated as the sum of molecular spectra: I will focus on models to describe J and H aggregates both in one and two dimensions, and calculate absorption and emission spectra. In the second part of the talk I will show how different molecules can interact at large distances (10-100 A) in the so called Förster Resonance Energy Transfer (FRET), in which the excitation can "jump" from a molecule (Donor), to another one (Acceptor) through non-radiative dipole-dipole coupling. Here I will present preliminary results of a Molecular Dynamics study with the aim of rationalize the role of slow degrees of freedom during resonant energy transfer mechanism.

Voditelj seminara:
Oleg Antipin
oantipin@irb.hr