



ELECTRONIC PROPERTIES OF DNA OLIGOMERS

A training ground for modelling and experiments

Room 27
Area della Ricerca del CNR di Pisa

Session 1:

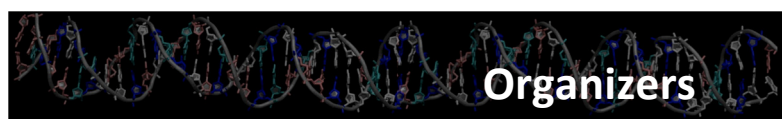
- 09:30 **D. Markovitsi (LIDYL-CNRS, U. PARIS-SACLAY)**
UV-induced properties in DNA studied by optical spectroscopy
- 10:10 **A. J. Pepino (U. BOLOGNA)**
Photoinduced decay of solvated pyrimidines nucleosides resolved at the CASPT2/MM level
- 10:30 **L. Martinez (IBB-CNR, NAPOLI)**
The photophysics of cytosine derivatives in solution
- 10:50 **C. Manzoni (IFN-CNR, MILANO)**
Pushing few-optical-cycle pump-probe and two-dimensional spectroscopy to the ultraviolet
- 11:10 **Coffee break**

Session 2:

- 11:40 **A. Peluso (U. SALERNO)**
Hole Transfer in DNA
- 12:20 **L. Esposito (IBB-CNR, NAPOLI)**
Insights on oligonucleotides from Molecular Dynamics simulations
- 12:40 **G. Brancato (SNS, PISA)**
A QM/MM molecular dynamics approach to DNA base tautomerism and microsolvation

Session 3:

- 14:30 **L. Blancafort (U.GIRONA)**
Computational studies of DNA chromophores: Cytosine derivatives and the ApU dimer
- 15:10 **I. Conti (U. BOLOGNA)**
A comprehensive analysis of the mechanisms leading to Thy-Thy photodimers in DNA double strand
- 15:30 **S. Jurinovich (U. PISA)**
Simulation of electronic circular dichroism of nucleic acids: from the structure to the spectrum
- 15:50 **J. Cerezo (ICCOM-CNR, PISA)**
Computational strategies to simulate the vibrational line shapes of biological complexes. Application to the CT rate in GC dimer



Roberto Improta, IBB-CNR
Fabrizio Santoro, ICCOM-CNR

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