



Martedì 9 dicembre 2025 alle ore 16:30 presso l'aula D del DiSC

Prof. Spiros S. Skourtis

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terrà un seminario dal titolo:

**Exploring the transport of electrons and excitons in
molecular and cellular systems via analytical-
computational models and ion-trap simulations**

La presenza della S. V. sarà molto gradita

Agostino Migliore

Il Direttore del Dipartimento
Stefano Mammi

Molecular electron and exciton transport processes are ubiquitous in biology and chemistry. These processes are also central to the development of molecular-scale electronics and of novel quantum and energy-harvesting materials. The molecular structures of chemical and biological electron/exciton transport systems have large structural variability. Due to this variability, overall transport distances and inter-molecular rates can vary over several orders of magnitude, depending on the underlying structures and reflecting different transport mechanisms. Fundamental questions to address are: (i) how molecular and electronic-vibrational structure and dynamics affect the transport mechanism (ii) how to control transport speed by modifying molecular structure and by applying external fields. I will describe some of my research work in this broad field: The simulation of electron transfer rates via ion-trap experiments, the modelling of very-long-distance hole transport in dry-DNA molecular junctions, the analysis of centimetre-scale charge transport in cable bacteria, and the design of molecular wires that sustain efficient long-distance triplet-exciton transport.

References

S Valianti, S.S. Skourtis

Activated electron transfer at zero reorganization energy induced by a fluctuating donor–acceptor coupling J. Chem. Phys. 162, 244116 (2025)

G. Polycarpou, S.S. Skourtis

Nickel-Dithiolene Cofactors as Electron Donors and Acceptors in Protein Hosts J. Phys. Chem. B. 129 (11), 9992-3006 (2025)

G. Polycarpou, S.S. Skourtis

Intra-strand phosphate-mediated pathways in microsolvated double-stranded DNA J. Phys.: Condens. Matter 36, 375301 (2024)

S. A. Mavrommati, S.S. Skourtis

Molecular Wires for Efficient Long-Distance Triplet Energy Transfer J. Phys. Chem. Lett. 13 (41), 9679-9687 (2022)

F. Schlawin, M. Gessner, A. Buchleitner, T. Schaetz, and S.S. Skourtis

Continuously Parametrized Quantum Simulation of Molecular Electron Transfer Reactions Phys. Rev. X Quantum 2 (1), 010314 (2021)