



Mercoledì **22 maggio 2024** alle ore **11:30** presso l'aula **F** del **DiSC**

Prof. Jochen Blumberger

Department of Physics and Astronomy, University College
London, London, UK

terrà un seminario dal titolo:

Charge and exciton transport in the transient delocalization regime

La presenza della S. V. sarà molto gradita

Agostino Migliore

*Il Direttore del Dipartimento
Stefano Mammi*

Charge transport in organic semiconductors has puzzled the experimental and theoretical community for several decades. Transport measurements on ultrapure organic crystals showed a decrease in the charge mobility with increasing temperature, a hallmark of band transport, while at the same time electron paramagnetic resonance and vibrational spectroscopy data suggested the existence of localized charge carriers hopping from one site to the next [1]. In the last ten years spectacular progress has been made in the theory and computer simulation of charge transport in organic semiconductors that has allowed us to reconcile and understand these puzzling observations at a molecular level, including transient localization theory [2], polaron transformed Redfield theory [3], finite temperature time-dependent density matrix renormalization group [4] and non-adiabatic molecular dynamics simulation [5]. In my talk I will explain the methodology we have introduced to propagate charge carriers in these materials, fragment orbitals based surface hopping, that has substantiated the view that transport in these materials occurs in a unique "transient delocalization" regime [6], mid-way between band and hopping. I will also explain how dynamic, structural and electrostatic disorder in thin films lead to localization [7] and how transient delocalization manifests in the thermoelectric transport of organic semiconductors [8].

[1] Troisi, A. Charge transport in high mobility molecular semiconductors: classical models and new theories. *Chem. Soc. Rev.* 2011, 40, 2347–2358.

[2] Fratini, S.; Mayou, D.; Ciuchi, S. The Transient Localization Scenario for Charge Transport in Crystalline Organic Materials. *Adv. Funct. Mater.* 2016, 26, 2292–2315.

[3] Balzer, D.; Smolders, T. J. A. M.; Blyth, D.; Hood, S. N.; Kassal, I. Delocalised kinetic Monte Carlo for simulating delocalisation-enhanced charge and exciton transport in disordered materials. *Chem. Sci.* 2021, 12, 2276.

[4] Li, W.; Ren, J.; Shuai, Z. Finite-Temperature TD-DMRG for the Carrier Mobility of Organic Semiconductors. *J. Phys. Chem. Lett.* 2020, 11, 4930–4936.

[5] Giannini, S. and Blumberger, J. Charge Transport in Organic Semiconductors: The Perspective from Nonadiabatic Molecular Dynamics. *Acc. Chem. Res.* 2022, 55, 819–830.

[6] S. Giannini, L. Di Virgilio, M. Bardini, J. Hausch, J. Geuchies, W. Zheng, M. Volpi, J. Elsner, K. Broch, Y. H. Geerts, F. Schreiber, G. Schweicher, H. Wang, J. Blumberger, M. Bonn, and D. Beljonne, Transiently delocalized states enhance hole mobility in organic molecular semiconductors. *Nat. Mater.*, vol. 22, pp. 1361–1369, 2023.

[7] L. Stojanovic, J. Coker, S. Giannini, G. Londi, J. Yan, G. D'Avino, D. Beljonne, J. Nelson, and J. Blumberger. Disorder-induced transition from transient delocalization to charge carrier hopping conduction in the non-fullerene acceptor O-IDTBR. *PRX* 14, 021021, 2024.

[8] J. Elsner, Y. Xu, E. D. Goldberg, F. Ivanovic, A. Dines, S. Giannini, H. Siringhaus, and J. Blumberger. Thermoelectric transport in molecular crystals driven by gradients of thermal electronic disorder," under review, 2024.

After being a postdoctoral researcher at the University of Pennsylvania (2004–2006) and a Royal Society University Research Fellow for several years, Jochen Blumberger has become a Lecturer at the Department of Physics and Astronomy of the University College London in 2009, and then a Reader in 2013. Since 2015 he is Professor of Chemical Physics in the same department. Since 2020, Prof. Blumberger is Co-Director of the Thomas Young Centre, The London Centre for the Theory and Simulation of Materials, and since 2022 the Head of Condensed Matter and Materials Physics at the Department of Physics and Astronomy of UCL.