Department of Physics
Condensed Matter Physics
Clarendon Laboratory, Parks Road, Oxford OX1 3PU

UNIVERSITY OF OXFORD

CONDENSED MATTER SEMINAR

Thursday 26 January at 14.30

"Excited-state interaction dynamics in semiconducting materials from first principles"

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Understanding excited-state dynamics in functional materials is essential in emerging applications, from energy conversion to quantum information science. In particular, associated transport and relaxation mechanisms are coupled to optical selection rules, directly related to the underlying material structure. In this talk, I will present our recent studies on excited-state processes in functional materials upon light excitation, using predictive computations based on many-body perturbation theory. Specifically, I will discuss the effect of material dimensionality and symmetry in organic molecular crystals and transition metal dichalcogenides. I will present our new approach to relate non-analytical discontinuities in the excitation energies with the early stages of excited-state propagation, and discuss their coupling to lattice vibrations. Finally, I will discuss the role of state localization due to atomic defects and heterostructure composition in these processes.

Host: Prof Marina Filip