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MSP02 - Theory and Modelling of Excited-State Properties in Solids and Nanostructures

Organizers: C. Attaccalite (CINaM, Marseille), P. Romaniello (LPT, Toulouse), E. Cannuccia (PIIM, Marseille), A. Berger (LCPQ, Toulouse)

Invited Speakers: Fabienne Michelini (IM2NP, Marseille), Francesco Sottile (LSI, Palaiseau)

Many of the phenomena that shape our modern world—light emission in LEDs, charge separation in solar cells, photocatalysis, radiation damage, quantum information processing, and ultrafast spectroscopy—are governed by excited states. Understanding these states requires us to move beyond static pictures and confront the dynamic interplay of electrons, nuclei, and electromagnetic fields.

Theoretical and computational approaches to excited states present unique challenges. Electron correlation, non-adiabatic couplings, spin-orbit effects, and strong light-matter interactions often play decisive roles. Over the past decades, remarkable progress has been made through a variety of methods — from *ab initio* many-body approaches that aim for quantitative predictive power, to Green's function techniques that directly access spectral and quasiparticle properties, to effective and model Hamiltonians that distill the essential physics of correlation, excitonic structure, or light-matter interaction. These complementary perspectives allow us to bridge conceptual understanding and computational realism.

This mini-colloquium aims to bring together the communities working on model Hamiltonians and *ab initio* approaches, fostering strong connections between theoretical advances and material properties. Particular emphasis will be placed on the development and application of theoretical and computational methods to study light-induced phenomena, electron spectroscopy, charge transport, coupling to phonon modes, and magnetic excitations.