

**Computing The Optical Response Of Molecular Materials:
From Nano To Device Scales**

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Advances in nanoscience and material science are accelerating the rate at which we can create new materials. But, quite often, experiments are ahead of theory due to the challenging multiscale and multidisciplinary character of the experimental systems. In my talk, I will present a novel methodology which, starting from ab initio quantum mechanical molecular simulations, allows one to compute the electromagnetic response of macroscopic photonic devices containing molecular materials. I will show several examples, including a study of the polaritonic structure of a molecular film inside an optical cavities, and the second harmonic generation of molecular monolayers on top of substrates.