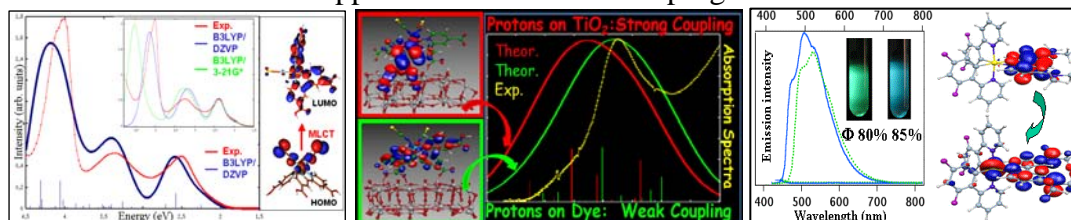


***Ab initio* simulation of the optical properties of nanoscale systems**

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Our group has a long-term and consolidated expertise in the computer simulation by *ab initio* methods of the structural, electronic, spectroscopic and non-linear optical properties of nanoscale systems and devices. We devised over time a computational strategy based on DFT and its Time Dependent extension (TDDFT) which allows the accurate calculation of excited state properties of large systems in solution. Our efficient implementation of the Car-Parrinello method,¹ allows us also to calculate the structures of realistic systems.^{2,3} Inclusion of solvation effects provides a direct connection of the calculated properties to the experimental quantities. Due to these methodological advances, theory is today a predictive tool, allowing us to scrutinize the properties of several species before their synthesis. An important characteristic of our group is the strong synergy with experimental investigations, with main applications in the field of OLED⁴⁻⁷ and DSSCs.⁸⁻¹⁴ In particular, we performed several calculations on the excited states of Ir(III), Fe(II) and Ru(II) complexes and organic dye-sensitizers. Realistic models of DSSC devices have then been obtained by adsorbing different dyes on TiO₂ nanoparticles,¹²⁻¹⁴ simulating the fundamental processes of light-harvesting and charge injection in DSSCs.¹⁴ Modelling of the optical properties of ZnO nanostructures and their application in DSSCs is in progress.



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