General conclusions and perspectives

The specific and general conclusions of each section have already been given in the respective chapters. Accordingly, the following lines are devoted to conclude this thesis in general terms and also present some perspectives for future work.

During this thesis, the essential knowledge on the field of molecular photophysics has been acquired. The understanding of molecular excited states has been in part achieved by the rationalization of experimental observations with electronic structure calculations. On the other hand, the review of past and recent literature on experimental and theoretical works has provided me with a broad perspective on this research field.

The results presented in this thesis show that the absorption and emission processes in the studied molecules can be properly described with the tools from quantum chemistry. The description of nonadiabatic processes, however, is more demanding. An investigation that naturally follows from the presented work is to explore whether the normal modes that dominate the Franck-Condon factors are somehow related to the nuclear motions that nonadiabatically couple electronic states.

The description of excited states in molecular crystals is still challenging from a computational viewpoint. The evaluation of structural models to properly represent the chromophoric units in the crystals is something to be addressed in a near future so to understand the experimental observations and reveal the dominant interactions in the solid state.

In addition, the molecular photophysics field remains to be nourished from the concepts of solid state physics so as to (i) develop new methods for treating phenomena in aggregates and crystals, and (ii) propose manageable qualitative models to describe the couplings between constituting units in the solid state.

By collaborating with experimental groups and reviewing the experimental literature it follows that there is a significant knowledge gap between the experimental and theoretical fields. In particular, recurrent interpretations of experimental observations seem to lack a theoretical justification. There still remains a lot of effort to be made in fundamental grounds, both from experimental and theoretical viewpoints, to justify many of the affirmations present in the literature.

Finally, the study of excited states seems to be one of the most promising fields in the near future of quantum chemistry. There are still many questions to be addressed and significant progress will surely take place in the following years. In the coming times, I hope to develop my scientific career in this field, studying the interaction between light and matter from a chemical and physical perspective.