A Biexciton Model for Exciton-Exciton Interactions in Para-hexaphenyl

Leonardo Evaristo de Sousa¹(PG), Fernando T. Bueno¹(IC), Pedro Henrique de Oliveira Neto¹(PQ) and Demétrio Antônio da Silva Filho¹(PQ) *leonardosousa@unb.br*

¹Institute of Physics, University of Brasilia

Biexcitons, exciton-exciton interactions, organic materials, kinetic Monte Carlo .

Introduction

At large concentrations, exciton-exciton interactions play an important role in the exciton dynamics in organic materials. These interactions may take the form of exciton-exciton annihilation or may even result in the production of biexcitons. Biexcitons usually have a very short lifetime and their recombination may also stimulate the emission of another photon in a process deemed biexciton cascade emission. These features are, thus, of high importance to the field of organic electronics.

In the particular case of para-hexaphenyl (P6P) films, experiments performed with different exciton concentrations have found evidence for the existence of both exciton annihilation and biexciton production. These two phenomena, however, present different results when considering the emission spectra of the material as well as its time-resolved photoluminescence spectra. Here we create a model for biexciton generation and exciton annihilation in P6P, study its consequences and compare the results to experimental data.

Methods

A Kinetic Monte Carlo (KMC) model was employed to simulate exciton dynamics. Site energies were chosen in order to reproduce the experimental emission spectrum of P6P. When excitons find each other in the material, they may either produce a biexciton, followed by the emission of two photons, or they may annihilate each other. Spontaneous emission is also taken into account. Time-resolved photoluminescence spectra are simulated for various concentrations. Decay times and amplitudes are obtained and their dependence on exciton concentration is investigated.

Results and Discussion

Results show a pronounced biexciton peak to appear as concentration becomes larger. The emission intensity shows a quadratic dependence on concentration, as expected for a two photon process and as experimentally obtained. Characteristic decay times are also obtained and are shown to decrease with concentration. The exciton-exciton interactions also reduce significantly the exciton diffusion length in the material. Temperature effects on exciton dynamics under large exciton concentrations are also studied.

Conclusions

In this study we simulate exciton dynamics in P6P films at high exciton concentrations. A model of biexciton production in conjunction with a KMC model account for some experimental results indicating that this phenomenon may be of importance in the functioning of optoelectronic devices produced with organic materials.

Acknowledgements

We gratefully acknowledge the financial support from CAPES and FAP-DF.

References

- Evaristo de Sousa, Leonardo, et al. "Biexciton cascade emission in multilayered organic nanofibers." *Applied Physics Letters* 112.14 (2018): 143301.
- de Sousa, Leonardo Evaristo, et al. "Modeling temperature dependent singlet exciton dynamics in multilayered organic nanofibers." *The Journal of chemical physics* 148.20 (2018): 204101.