15a

Advisor: **Dr. Gabriel Ramos Ortiz**

Committee Members:

Dra. Laura Elena Casandra Rosales Zárate
(Secretary)

Dr. Roberto Ramírez Alarcón
(Evaluator)

Dr. Gabriel Ramos Ortiz
(Chairperson)

Thesis: "GENERAL STUDY OF CLASSICAL AND NONCLASSICAL CONTRIBUTIONS OF TWO PHOTON ABSORPTION PROCESS IN ORGANIC MOLECULES"

Summary:

Since the discovery of black phosphorene (a monolayer of bulk black phosphorus), new 2D allotropes of phosphorus have been predicted and studied due to their interesting properties. Some possible applications of these phosphorene structures could be in photovoltaic cells, gas sensors and rechargeable batteries. In particular, blue phosphorene is characterized by having a hexagonal structure, and thus, an isotropic optical response on the plane of the layer structure. The electronic band structure of blue phosphorene was obtained by using Density Functional Theory within the Generalized Gradient Approximation. It is observed, based on its band structure, that blue phosphorene shows a semiconducting nature, with an indirect band gap. The energy corrections to the bands were calculated in a specific set of k points within the irreducible Brillouin zone by employing the GW approximation and the complete quasiparticle band structure was determined by using maximally localized Wannier functions. The comparison between Generalized Gradient Approximation and GW calculated band structures shows that there are significant differences, which demonstrates the importance of performing quasiparticle corrections. In general, neither the calculation of the optical spectrum in the independent-particle approach nor the calculation using the the quasiparticle energies obtained in a GW correction match correctly the experimental data of the absorption of the materials. Therefore, the optical response including excitonic effects (electron-hole interactions) has to be calculated. For that, the excitonic spectrum is obtained and compared with both the independent-particle and GW optical response.