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Director de tesis: Dr. Bernardo Mendoza Santoyo

Sinodales: Dra. Laura Elena Casandra Rosales Zárate
(Sinodal Interna, Secretaria)

Dr. Joel Briones Hernández
(Sinodal Interno, Vocal)

Dr. Bernardo Mendoza Santoyo
(Director de Tesis, Presidente del Jurado)

Tesis: **"AUTOMATED PROGRAM FOR THE CALCULATION OF THE QUASIPARTICLE ENERGIES WITH THE GW APPROXIMATION"**

Resumen:

This thesis presents a general description of a program that automatizes the calculation of the quasiparticle energies of crystalline systems, by using the GW approximation. In this context, G is a Green's function that describes the dynamic of an electron. W is the dynamical screen interaction between electrons in a homogeneous and polarizable medium. The automation of the program consists in computing important functions that are needed to calculate the quasiparticle energies. These functions are the charge density, wave functions, the polarizability and the self-energy. All these functions can be computed by the software Abinit. However, the computation of those functions are not automatized by Abinit. The program developed in this thesis allows one to compute the eigen-energies of the system by using Density Functional Theory, and the Local Density Approximation for exchange-correlation potential Vxc. The program calculates quasiparticle energies and the optical band of semiconductors. The program also calculates the quasiparticle energies, Fermi energy and spectral function of metals. We calculated the linear dielectric function with the quasiparticle energies, by using the Random Phase Approximation for polarizability. The results show that the linear dielectric function computed with the quasiparticle energies is in agreement with experiments for semiconductors. The results also show that the optical band gap computed with GW approximation is more precise respect to experiments, in comparison with the optical band gap predicted by the Density Functional theory.