SOUTENANCE DE THESE

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Numerical design of meta-materials for photovoltaic applications

The purpose of the thesis was to simulate the absorption spectrum of meta-materials for photovoltaic applications. By meta-material, we mean an assembly of nanometric size objects at mesoscopic distance. The underlying idea is that by adjusting the size of the nano-object and the geometric arrangement, one could tune the absorption edge. To calculate these quantities, I used state-of-the art formalism, namely ab-initio methods.

The first part of the work has been dedicated to the calculation of the absorption of an isolated object (slab of silicon, graphene, hBN). In the framework of periodic codes, one uses a supercell with vacuum to isolate the object. A method was developed previously in the Theoretical spectroscopy group at LSI to provide results independent of vacuum : the "Selectd-G" method. It was successfully applied to silicon surfaces. For an isolated slab, the formalism has to be modified, using a slab potential. The Electron Energy Loss spectra for slabs of few graphene layers have been simulated, and successfully reproduced available experimental data. This has also offered the possibility to study the plasmon dispersion of a single graphene layer, and discuss the nature of electronic excitations in the system (interband transitions or 2D-plasmon).

The second step has been dedicated to the study of the absorption spectrum of an array of interacting slabs. The TDDFT, due to the repetition of the supercell contains the physical information. Since it has been evidenced that the supercell formalism acts as an effective medium theory with vacuum, with the spurious effect of having spectra dependent on the size of the supercell, I have reversed the procedure to extract the spectrum of the interacting slab, "cured" from the vacuum problem. The validity of this approach has been demonstrated on different kind of slabs, such as hBN or silicon slabs, showing an enhancement of the absorption at low energy due to surface states.

In the third part, I studied materials currently used or candidates for photovoltaic applications: InP and InSe. I have first studied the electronic structure of InP and InSe bulk, using hybrid Heyd-Scuseria-Ernzerhof (HSE) functionals, to correct for the underestimation of the band gap in the local density approximation (LDA). The absorption spectra have been calculated using the Bethe-Salpeter formalism to account for the excitonic effects and compared to the results with the much lighter calculation using TDDFT with a long range kernel to mimic the excitonic effects. I have started the calculations for slabs of these two materials. A 2x2 reconstruction have been performed for the InP slab to recover the semi-conducting surface. A InSe slab with 2 layers has been modeled. The absorption spectra have been calculated, within TDDFT for the isolated and interacting slabs.

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