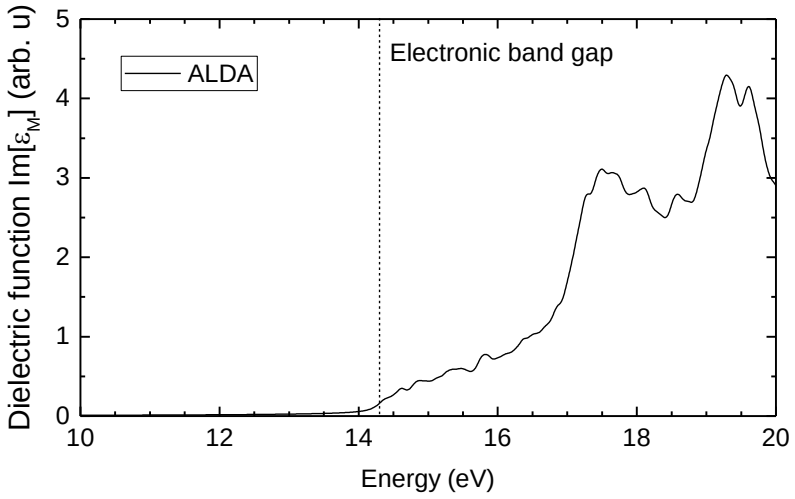
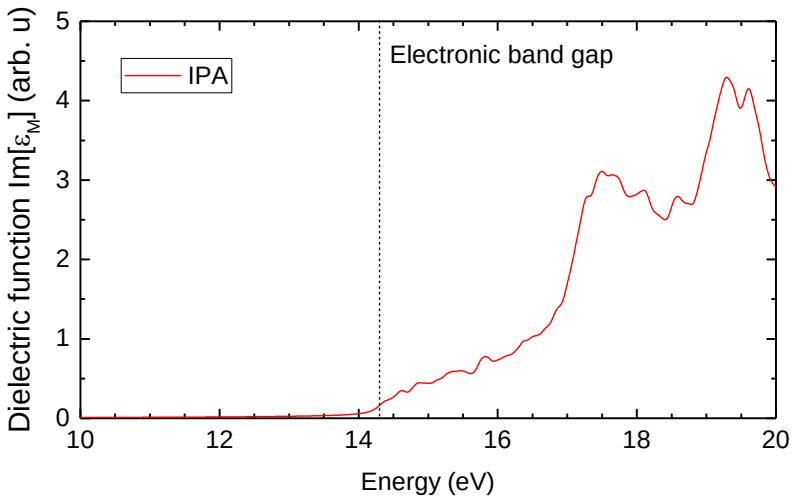
Solutions for excercise sheet 7

Exercise 1: TDDFT for absorption spectra

(a) Nothing to plot

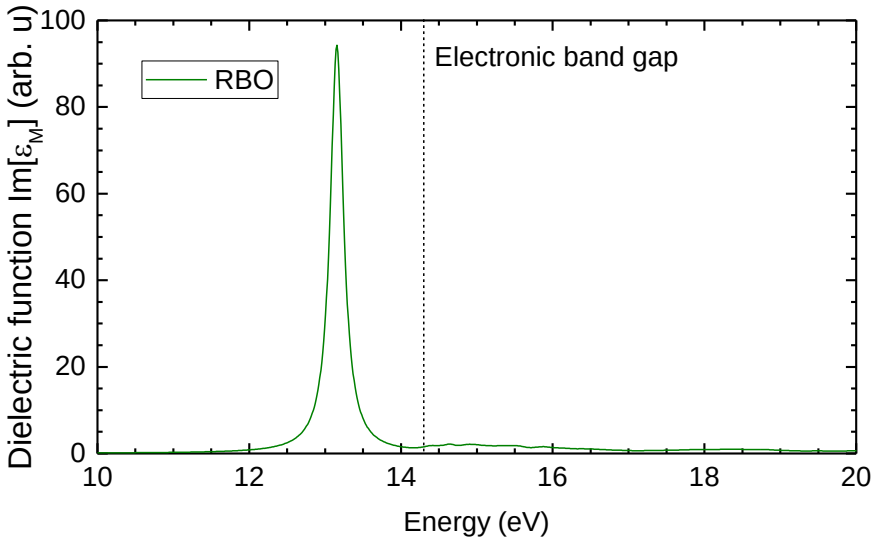
(b)





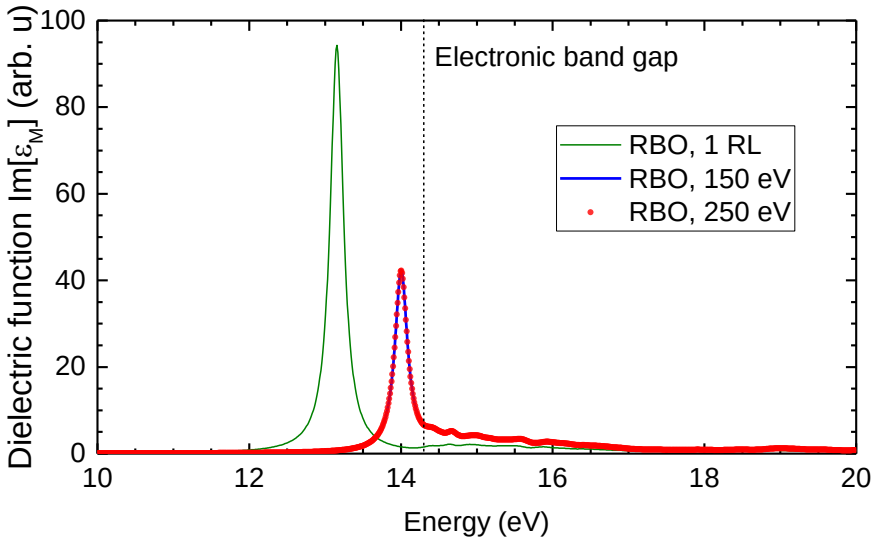
The exciton binding energies for these approximations are essentially zero, as the first “peak” appears at the energetic position of the electronic band gap. As we neglect all local field effects, the ALDA and RPA are equivalent to the IPA.

(c)



The exciton binding energy in this case is predicted to be about 2.1 eV.

(d)

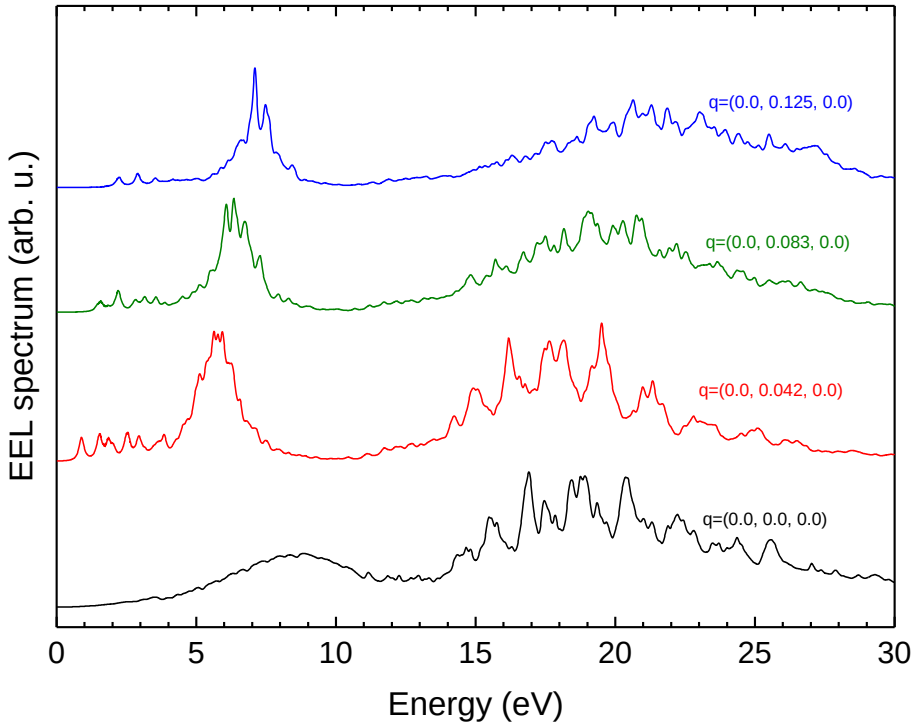


The inclusion of local field effects maintains the excitonic peak, but reduces the exciton binding energy (0.3 eV) and the optical oscillator strength of the excitonic peak. The new exciton binding energy is much smaller than the one obtained from experiments (>2 eV). A cutoff energy of 150 eV yields converged results (note that technically one could converge the cutoff for the Hartree part and that of the f_{xc} part independently).

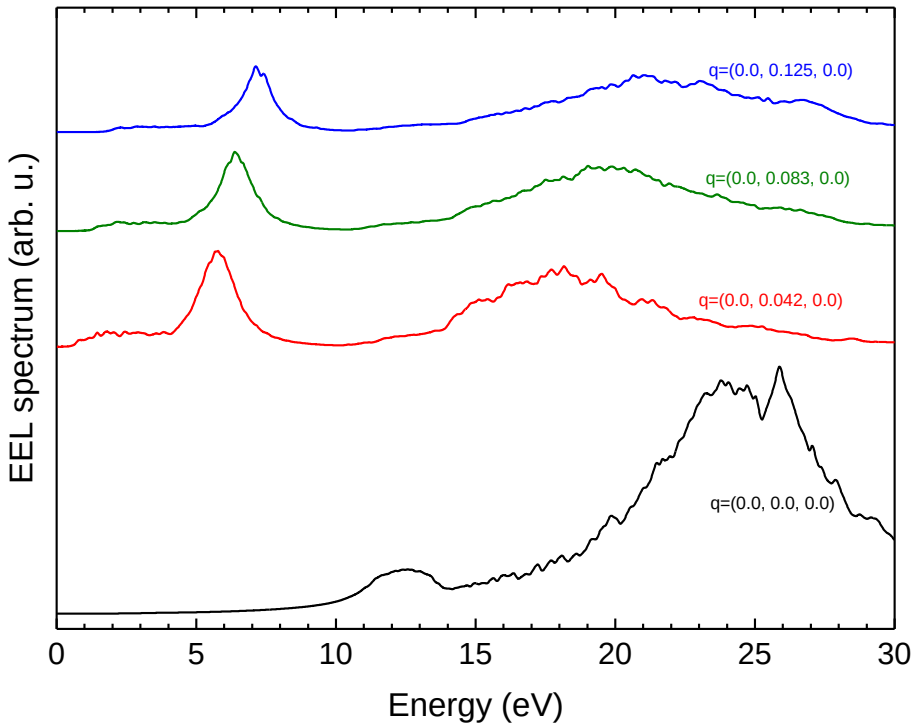
Exercise 2: Plasmon dispersion in Graphene

(a) Nothing to plot

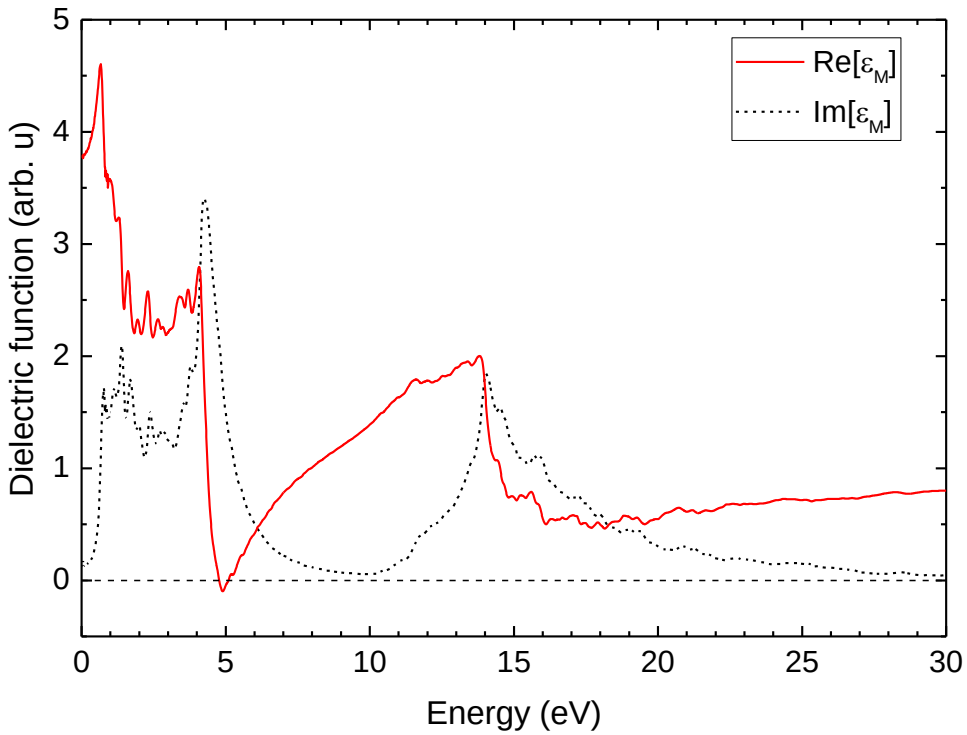
(b)



(c)



(d)


Re[ε_M]
Im[ε_M]
Dielectric function (arb. u)
Energy (eV)
0
1
2
3
4
5
0
5
10
15
20
25
30