Abipy/lumi/deltaSCF.py

Δ SCF post-process (1D)

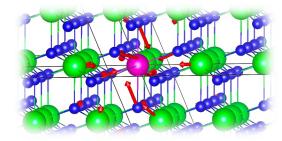
• Transition energies, Huang-Rhys factor, eff. phonon freq., ...

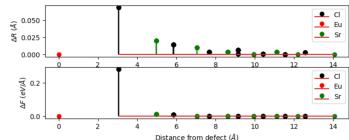
 E_em
 E_abs
 E_zpl
 E_fc_gs
 E_fc_ex
 Delta_S
 Delta_R
 Delta_Q

 site_1
 1.561313
 1.820608
 1.708639
 0.147326
 0.11197
 0.259296
 0.182233
 0.897472

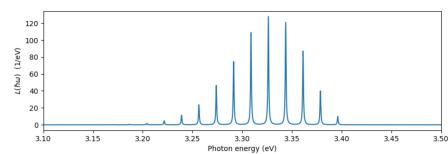
 $E_{Abs}=1.82 \text{ eV}$ $E_{abs}=1.82 \text{ eV}$ $E_{FC,g}=0.15 \text{ eV}$ $E_{C,g}=0.15 \text{ eV}$ $E_{C,g}=0.15 \text{ eV}$ $E_{C,g}=0.15 \text{ eV}$

• Atomic relaxation analysis





• Luminescence lineshape (1D model)



• Abinit output files (netcdf) from LumiWork

