LITESOPH

Layer Integrated Toolkit and Engine for Simulations of Photo-induced Phenomena

Tutorial Day 2

We have already learnt how to calculate photo-absorption spectrum using LITESOPH. Now, we will learn some further applications of the tool.

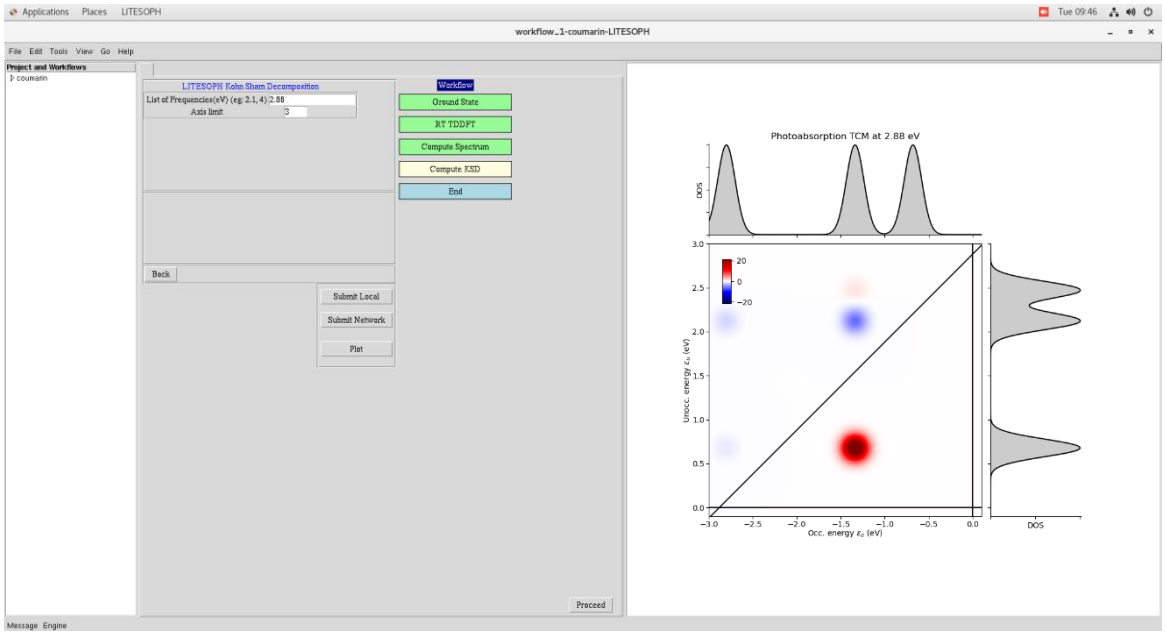
Kohn Sham Decomposition:

Rossi et al. have developed KS decomposition (KSD) tool based on the RT-TDDFT code that uses the linear combination of atomic orbitals (LCAO) method and enable calculations involving hundreds of noble metal atoms. In order to analyze the response in terms of the KSD, the decomposition is presented as a transition contribution map (TCM), which is an especially useful representation for plasmonic systems in which resonances are typically superpositions of many electron-hole excitations. The TCM represents the KSD weight at a fixed energy of excitation in the two-dimensional plane spanned by the energy axes for occupied and unoccupied states.

Launch litesoph gui, select Kohn Sham Decomposition in workflow.

After spectrum calculation, choose excitation energies to plot TCM.

Kohn Sham Decomposition



Output from KSD at 2.88 eV:

Frequency: 2.88 eV

Folding: Gauss (0.10000 eV)

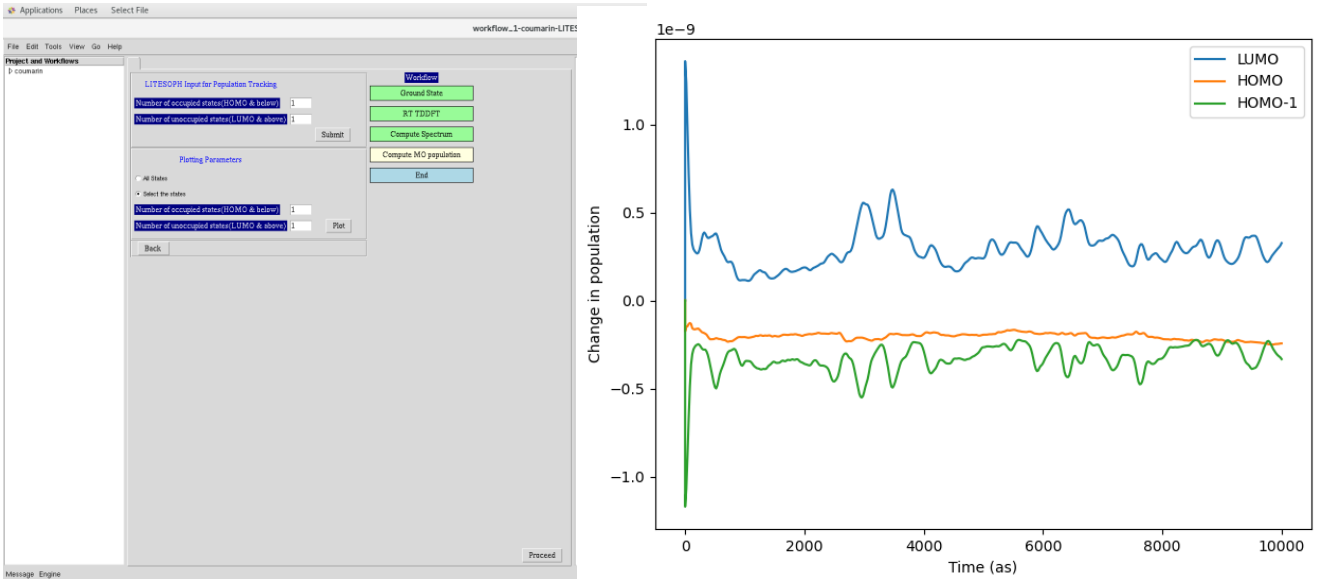
Total absorption: 0.76 eV^-1

#	p	i(eV)		a(eV)	Ediff (eV)	weight	%
1	25(	-1.336) ->		27(0.678):	2.0140	1.6882	221.4
4	25(	-1.336) ->		28(2.122):	3.4578	-0.3939	-51.7

9	24(-2.800) ->	28(2.122):	4.9217	-0.1117 -14.6
56	22(-4.061) ->	30(4.473):	8.5337	-0.1084 -14.2
		rest:	-0.3117	-40.9
		total:	+0.7625	100.0

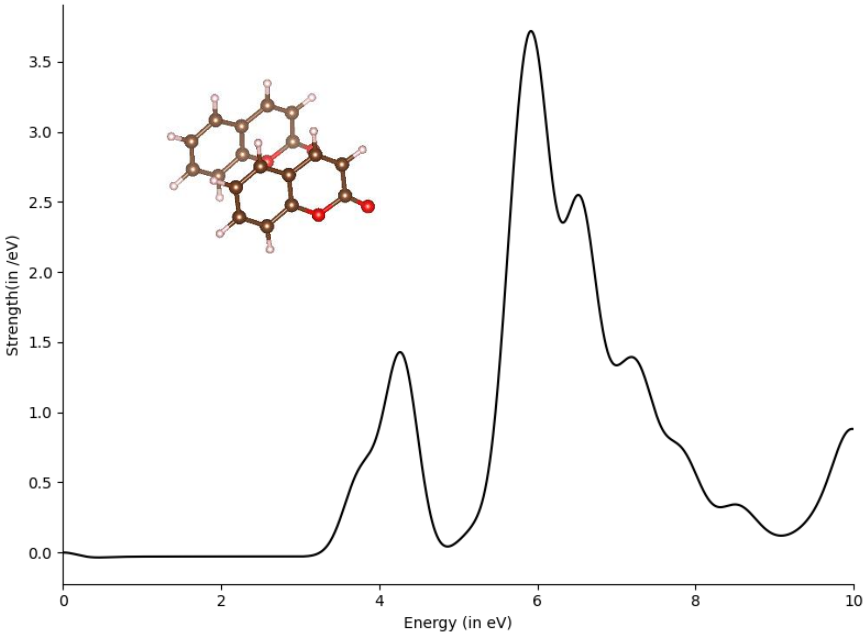
It shows that the lowest energy excitation is the excitation from 25 (HOMO-1) to 27 (LUMO).

MO Population Calculation:



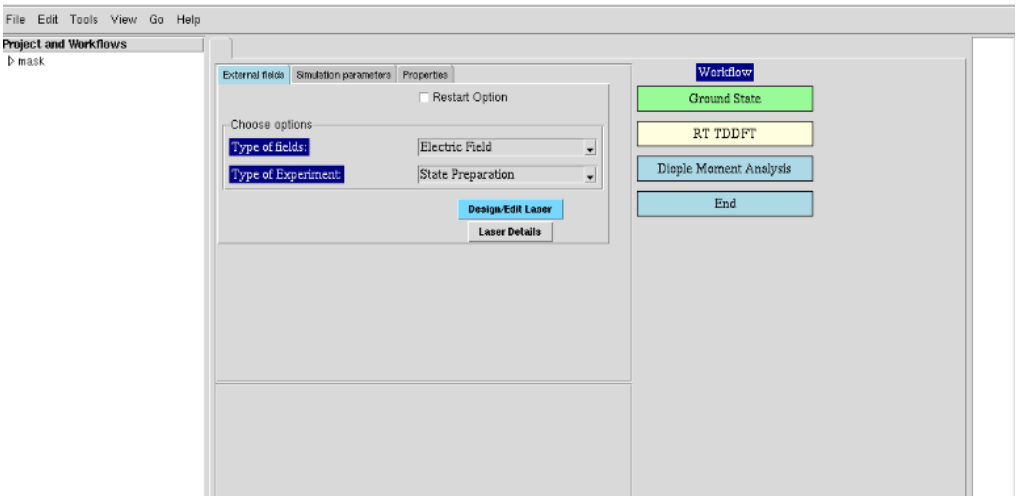
As it is clear from the MO population plot, the population of HOMO is constant while the population of HOMO-1 and LUMO is changing with time. It verifies that the excitation is happening from HOMO-1 to LUMO.

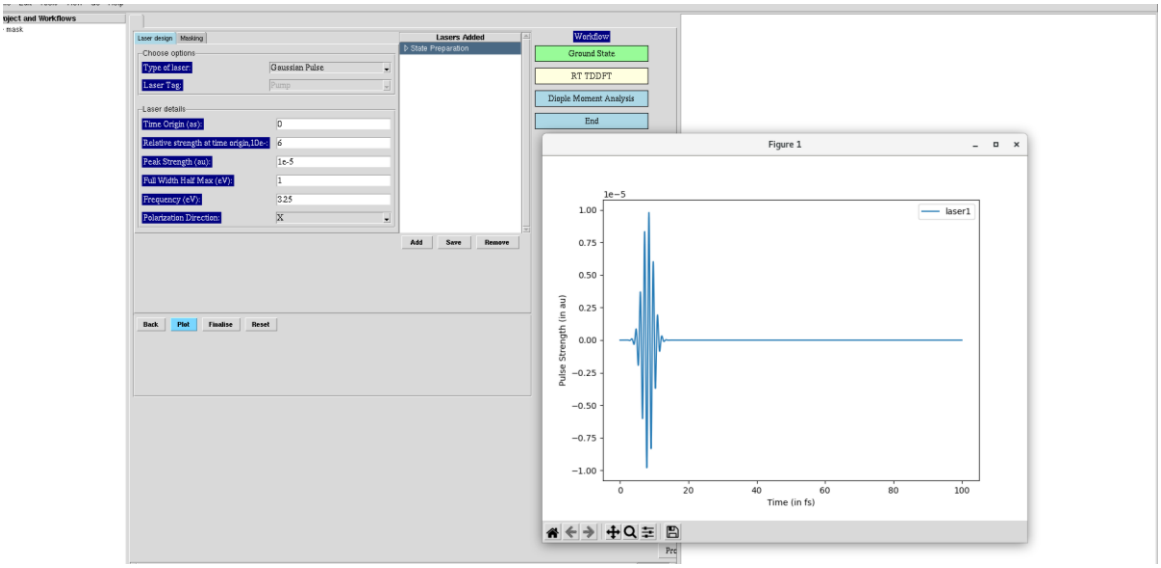
Coumarin-dimer:

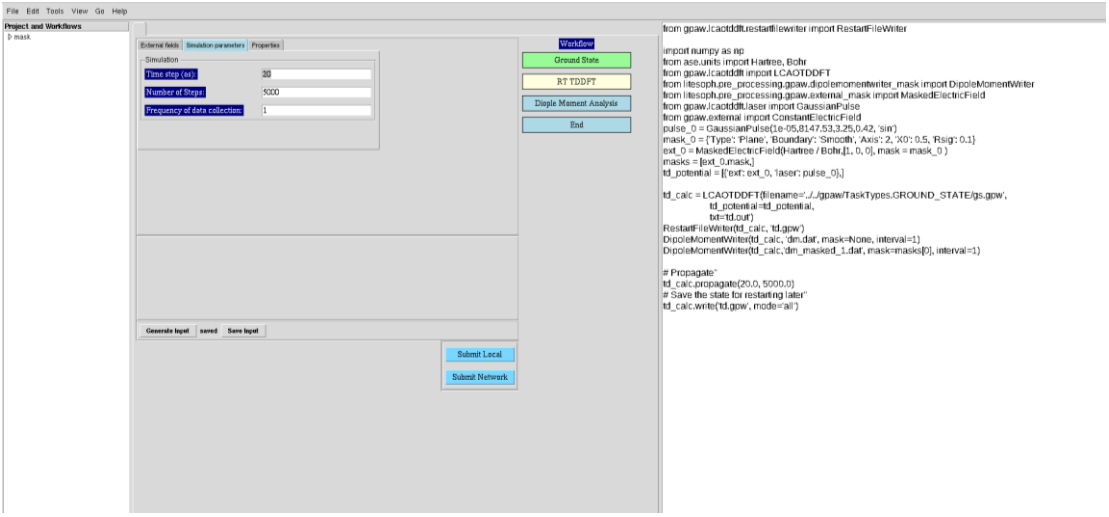


Photoabsorption spectrum of Coumarin-dime

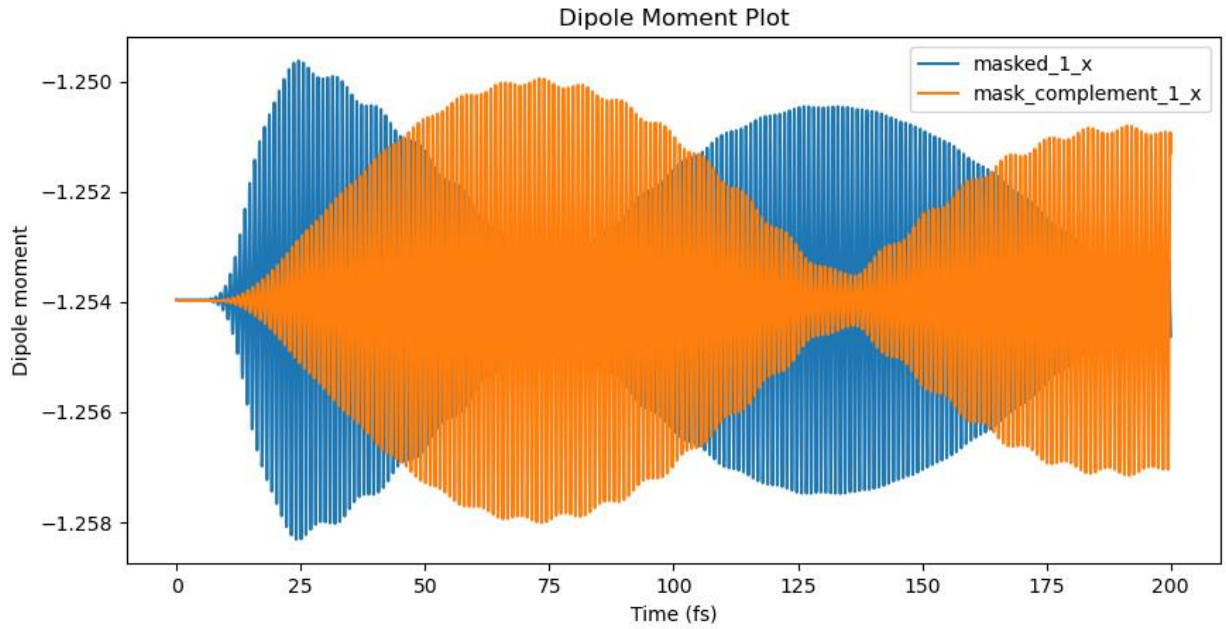
State preparation for masking:







Dipole Moment Analysis:



TD dipole moment of Coumarin-dimer

Energy Transfer Coupling Constant:

Region/Mask_Index	Focus_Value	Direction	Energy_Coupling(in eV)
mask_complement_1	False	y	0.337

Exercise:

Calculate energy transfer coupling constant for Coumarin-Bodipy hetero molecule.