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Use case: Influence of enviromental effects on excitation spectra of host materials

Introduction

Quantum mechanical methods such as DFT or TD-DFT are widely used to calculate the electronic properties of single molecules or pairs. However, in organic electronics, molecules are usually embedded in layer structures that create a unique electrostatic environment for each molecule. This modifies the electronic properties such as energy levels or excitation energies uniquely for each molecule, making the calculation of isolated compounds or pairs in vacuum unreliable.

This use case demonstrates how QUANTUMPATCH is applied to the calculation of excitation spectra of three host materials. Environmental effects are taken into account on full quantum mechanical level.

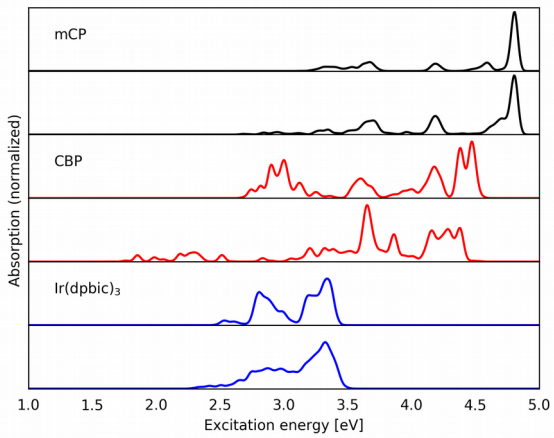
The results were derived using three steps:

1. Single molecule parametrization using the PARAMETRIZER
2. Generation of molecular layers consisting of 1000 molecules with atomistic resolution for three different molecules (mCP, CBP, $Ir(dpbic)_3$) using DEPOSIT
3. Excitation spectra were generated by calculating the 30 lowest excitations for each molecule in the structure using QUANTUMPATCH (with TD-DFT engine as implemented in Turbomole) and computing the average.

Detailed parameters for each step are given below.

Results

Excitation spectra are displayed in the figure to the right for mCP (red), CBP (red) and $Ir(dpbic)_3$ (blue). Excitation spectra calculated including environmental effects using QUANTUMPATCH (lower lines) are compared to the excitation spectra of molecules in vacuum (upper lines).



Especially for CBP and Ir(dpbic)3, excitation spectra change significantly when the molecules are placed inside amorphous layers. To achieve reliable results it is therefore essential to include the unique molecular environment on full quantum mechanical level, e. g. with QUANTUMPATCH. This does not only apply to excitation spectra, but any electronic property such as HOMO or LUMO energy level, electronic coupling of pairs or charge transfer processes.

Parameters used in the calculation:

Parametrizer:

Geometry optimization	DFT (B-P, def2-SV(P))
Partial charges	DFT (B-p, def2-SV(P))
Dihedral parametrization	semiempirical (PM6)

Deposit:

Number of molecules	1000
Number of SA cycles	10
Number of steps per cycle	140.000
Initial temperature	4000K
Final temperature	300K

QuantumPatch:

No. of Mol in inner shell	20
No. of partial charge steps	7
Method	TD-DFT, b-p, def2-SV(P)
No. of excitations	30
Hybrid mode	On