

Optical property of possible candidates from CEPDB database

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1. Database

Registration is needed to search and see the top candidates.

For our purpose, search can be done using the SMILE formula

In this input here, **the atoms in the rings should be in lower case**. Otherwise, the engine couldn't find it.

Solar Cell PerformancePrincipal Energy LevelsName & SubstructureSearch Settings

SMILES (Simplified Molecular-Input Line-Entry System)

☐ Exact search

This field is case sensitive but accepts both complete and partial SMILES. Molecule can be sketched and their SMILES obtained with Marvin. Note: aromatic rings are in lower case.

Stoichiometric formula

☐ Exact search

Partial or complete stoichiometric formula.

Mass

min, in amumax, in amu

SEARCH

Start over

2. Search in the database

a. Search the whole molecule

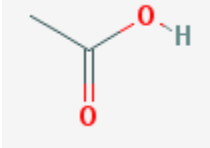
DHICA	<chem>c1=c2c=c(nc2=cc(=c1O)O)c(=O)O</chem>		None
3-phenyl-DHICA	<chem>c1=cc=c(c=c1)c2=c(nc3=cc(=c(c=C32)O)O)c(=O)O</chem>		None

b. Search the fragment

Indole	<chem>c1=cc=c2c(=c1)c=cN2</chem>		None
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Phenol	<chem>c1=CC=C(C=C1)O</chem>		None
Eugenol	<chem>cOc1=c(cc(=c1)C=C)O</chem>		None

c. Search the function group

Carboxylic acid	<chem>CC(=O)O</chem>		None

d. Observation of top 1000 compound

- All of them have one Sulfur atom or more. Most of them have Silicon atom. Many of them have Se atom.
- Nearly all of them form ring structure.

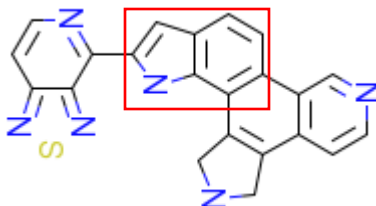
e. Identify the Indole group from the top 1000 compound. (doing it)

- Feature: 5-atom ring with one N, connect to 6-atom ring.
- Problem:
 - The SMILES for Indole changes in different compounds? (Counting start point different?)

f. The Abs spectra of top compounds

- Calculate the “c1[nH]cc2c1c1ccncc1c1ccc3cc([nH]c3c21)-c1nccc2nsnc12”

(<https://cepdb.molecularspace.org/single/c1%5BnH%5Dcc2c1c1ccncc1c1ccc3cc%28%5BnH%5Dc3c21%29-c1nccc2nsnc12>)



Computational Results & Predictions

Principal Energy Levels

ϵ_{HOMO} [eV]	ϵ_{LUMO} [eV]	ϵ_{gap} [eV]
-5.41	-4.00	1.41

Photovoltaic Performance Parameters

PCE (Power Conversion efficiency [%])	V_{oc} (Open-Circuit Voltage [V])	J_{sc} (Short-Circuit Current Density [A/m^2])
11.12	0.81	210.89

3. Workflow:

Step1. Geometry opt using Gaussian09. (B3LYP/6-31++G(d,p))

Python script for this step: generate_G09_input_from_html.py:

Generate structure from the html from the website;

Initial optimization using pybel;

Using steepest Descent to opt the structure

Save as mol_name.pdb file

Shell script: submit09:

Use the template to generate the input file

Submit input file to Gaussian09 for optimization

Step2. gs calculation using octopus

Python script for this step: extract_G09_output_to_xyz.py

Gaussian09 output extraction and save as *.xyz file.

Shell script for this step: submit_gs

Set up a folder called "gs" in the HPC and copy the *.inp file there.

Modify the coordinate's part by adding:

```
XYZCoordinates = "mol_name.xyz"
```

Submit the input file

Step3. td calculation using octopus

Shell script for this step: submit_td1:

Set up 3 folders called td_x, td_y and td_z. Copy all the content from the gs folder to td_x, td_y and td_z, respectively. Then in their td inputs, change the direction to be x, y and z, respectively. This can be done by using:

```
TDPolarizationDirection = 1
```

Step4. Calculation of cross section/absorption

Shell script for this step:

Copy the multiple in the 3 folder and rename them into multiple.1, multiple.2 and multiple.3.

Upload them to the ps057-vaquero. Use utility :

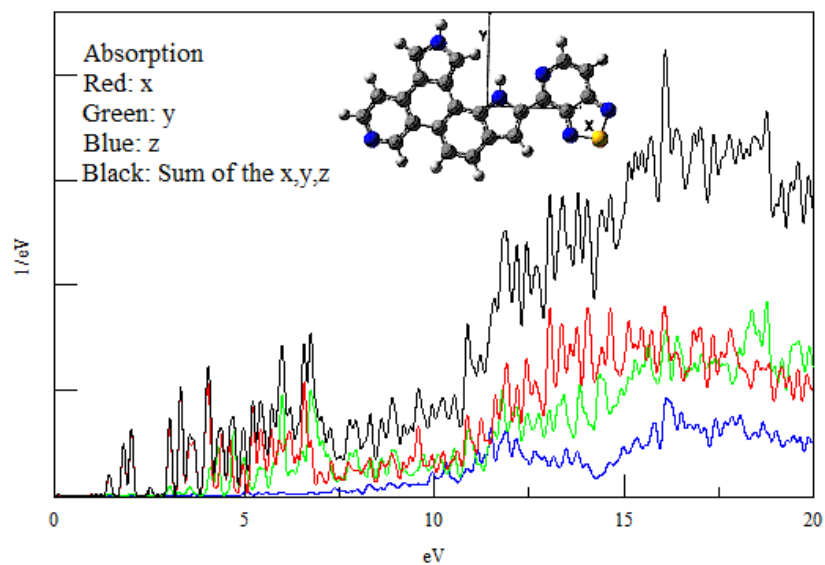
```
/state/partition1/apps/bin/oct-propagation_spectrum
```

Step5. Plot the absorption spectra:

X: first column in the cross_section_vector;

Y: 5-th column in the cross_section_vector;

Sum of 3 direction: add x, y and z together.



41 atoms	G09 optimization	Octopus gs	Octopus td_x	Octopus td_y	Octopus td_z
Time used	186m	54m	3201m	2465m	2577m

4. Template for the input file:

a. for step 3, octopus (ground state part)

```

Units = eV_angstrom
CalculationMode = gs
Theorylevel = DFT

Spacing = 0.20
BoxShape = minimum
# The radius can be set based on the recommendation in the pseudo potential  setting it
at 5 overrides that
# Radius = 5.00

XCFunctional = hyb_gga_xc_b3lyp

fromScratch = yes
# -----
# TD RUN Parameters
# -----
TDDeltaStrength = 0.01
TDPolarizationDirection = 1

# 1 fs = 1.519 time unit
# 1 time unit = 0.658 fs

# The time needed might not be as large. Especially if you are to use the compressed
sensing

# 25fs
stime = 38.0

dt = 0.0025
TDPropagator = aetrs
TDEXponentialMethod = taylor
TDEXponentialOrder = 4
TDLanczosTol = 5.0e-5
TDMaximumIter = stime/dt
TDTimeStep = dt
OutputEvery = 500

# -----
# Spectrum Parameters
# -----

# ExperimentalFeatures = yes
# SpectrumMethod = compressed_sensing
# SpectrumSignalNoise = 0.0001

# Change this number, if we want smaller perturbation time
# PropagationSpectrumEndTime = 3.7975

```

b. for step 3, octopus (TD-DFT part: x-direction)

x-direction: add TDPolarizationDirection = 1

y-direction: add TDPolarizationDirection = 2

z-direction: add TDPolarizationDirection = 3

```
Units = eV_angstrom
CalculationMode = td
Theorylevel = DFT
```

```
Spacing = 0.20
BoxShape = minimum
# The radius can be set based on the recommendation in the pseudo potential setting it at 5 overrides that
# Radius = 5.00
```

```
XCFunctional = hyb_gga_xc_b3lyp
```

```
fromScratch = yes
# -----
# TD RUN Parameters
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```
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# -----
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