

LDA OPT

Required Files

- compound/output/compound.absorp
compound may be shorthand

Function

read .absorp file

Data description (label) is found in line containing “Energy [eV]”

Headers are found in lines containing “#”

Data is in columns

Only record data with “sigma” in the description

Append each column to a data object

Data object records plot data (numbers), index (column number in .absorp), and equation (description of data)

Output

Visual plot generated from data

Searches for specific data sets are based on index and equation

X,Y axis can be modified

Grid can be applied

Data also is presented in files

Data files exist for one week from the time of creation

name of file: ldaoPT EQUATION.txt

format of data file:

1st column: x-data

2nd column: y-data