

I have the following equation:

$$E = \left[16 \pi^2 (13.605)^2 \right] \times \frac{1}{(\text{eig})^2} \times \sum (\text{Dip}_-)^2 \times \text{Delta}$$

I need to get some values from the following txt file (eigenvalue_nosh.dat) in support of the above equation:

File:

										ω (eV)	
1	# neig =	777600									
2	# vol =	0.630490974E+05									
3	# nspin, nkpt, ncb, nvb =										
4	#	ik	ic	iv	is	ec (eV)	ev (eV)	eig (eV)	abs(dipole)^2	dipole	
5		1	1	1	1	0.73760347E+02	0.36820680E+02	0.36939667E+02	0.37700076E-02	0.61400388E-01	
6		1	1	2	1	0.73760347E+02	-0.33100160E+02	0.10686051E+03	0.41246494E-04	-0.64223434E-02	
7		1	1	3	1	0.73760347E+02	-0.33104646E+02	0.10686499E+03	0.17556626E-03	0.13250142E-01	
8		1	1	4	1	0.73760347E+02	-0.33109496E+02	0.10686984E+03	0.24123677E-01	-0.15531799E+00	
9		1	1	5	1	0.73760347E+02	-0.36816821E+02	0.11057717E+03	0.91220666E-02	0.95509510E-01	
10		1	1	6	1	0.73760347E+02	-0.36826440E+02	0.11058679E+03	0.70405477E-02	-0.83907972E-01	
11		1	1	7	1	0.73760347E+02	-0.36831833E+02	0.11059218E+03	0.76894401E-03	0.27729840E-01	
12		1	1	8	1	0.73760347E+02	-0.71827464E+02	0.14558781E+03	0.25098104E-04	-0.50098007E-02	

Also:

$$\text{Delta} = 1, \text{ if } ec - ev = eig$$

$$= 0, \text{ if } ec - ev \neq eig$$

$$\text{Dip}_- = \text{Dip} \cdot \text{Gaussian}$$

$$\text{Gaussian} = \frac{1}{0.5 \sqrt{2\pi}} \cdot e^{-\left[\frac{(X - eig)^2}{2 \cdot (0.5)^2} \right]}, \text{ if } eig = ec - ev$$

$X \rightarrow$ x axis, all values from 0 to 500

Now, I need to have a python script to plot E vs X

