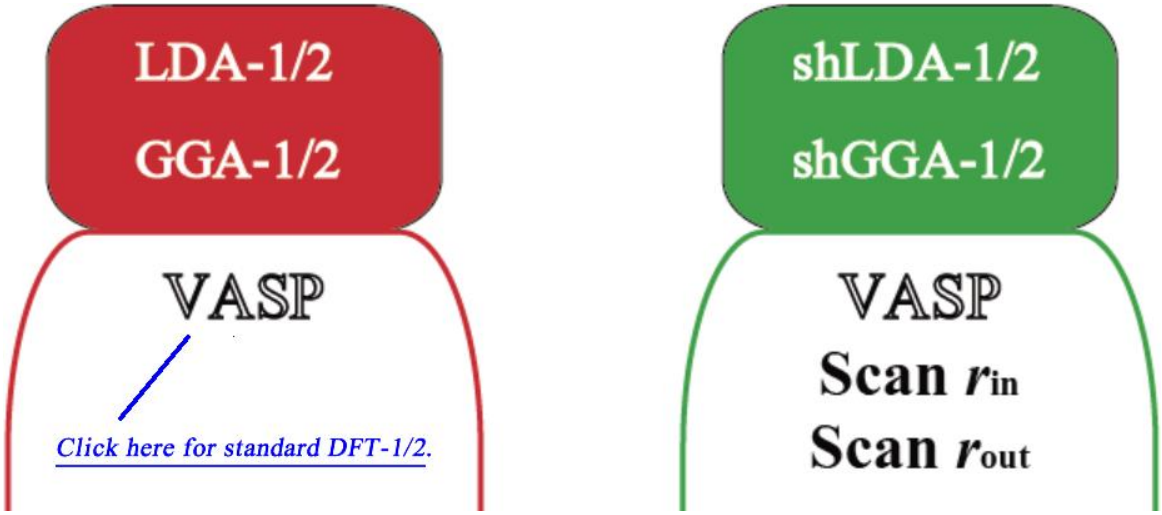
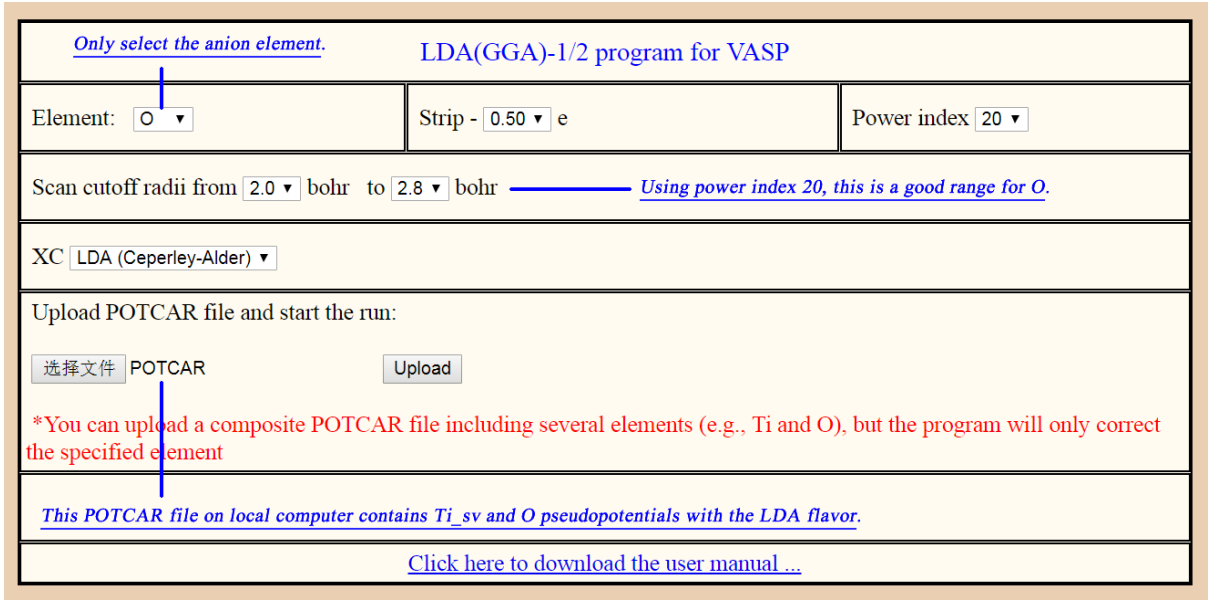
User Manual for online DFT-1/2 or shDFT-1/2 corrections

---- For VASP

1. Visit http://www.eedevice.com/dft-half/



2. Select DFT-1/2 input settings as shown below. We use LDA-1/2 calculation for rutile TiO_2 as an example. For oxygen, using power index 8 or 20, the typical optimal cutoff radius is 2.7 bohr or 2.3~2.4 bohr, respectively. Click "Upload" triggers the online calculation.



The uploaded POTCAR file contains Ti_sv and O pseudopotentials:

PAW Ti_sv 26Sep2005

12.0000000000000

… …

End of Dataset

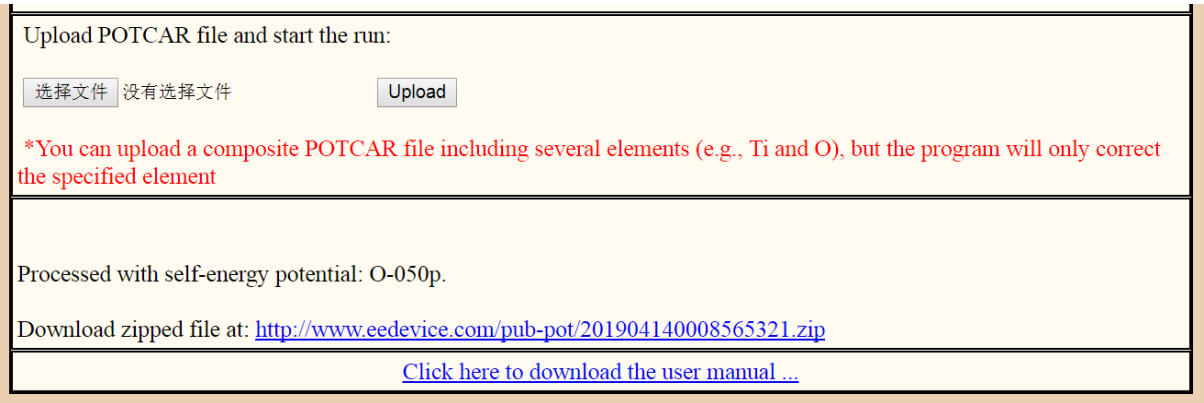
PAW O 22Mar2012

6.00000000000000

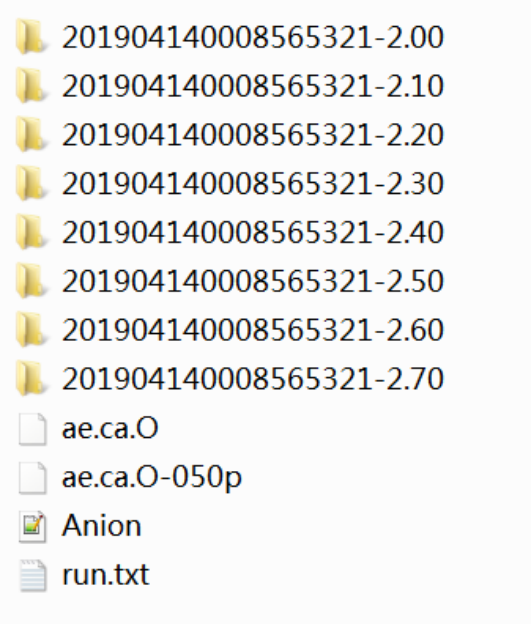
… …

End of Dataset

3. After a short while, the webpage will refresh and afford you a zip-format output file. Download it to local computer.



4. Unzip this file and you will obtain the following files:



Here the two "ae.*" files are the all-electron potentials for the neutral atom and the half-electron-stripped ion, respectively. The "Anion" file contains the pseudopotential of the anion element before self-energy correction. The "run.txt" file includes some parameters regarding this DFT-1/2 run. All these files are just for your information. The remaining folders ending up with the cutoff radius (unit: bohr, or a. u.) are the key outputs. Each folder contains a self-energy corrected POTCAR pseudopotential file, which also includes both Ti_sv (uncorrected) and O (corrected) in our example.

5. Copy INCAR, KPOINTS and POSCAR files into each folder, and run VASP for each folder, respectively.

   Typically these folders need to be uploaded to Linux servers for VASP calculation. You can write scripts using Bash or Python to copy the other three files automatically.

6. Compare the band gap values obtained using various anion self-energy potential cutoff radii. Here we obtain:

Cutoff (bohr)	Band gap (eV)
2.00	3.002855
2.10	3.074167
2.20	3.129049
2.30	3.162263
2.40	3.171549
2.50	3.153162
2.60	3.098784
2.70	3.013654

The maximum band gap (3.17 eV) is obtained using a 2.40 bohr cutoff radius.

7. Copy the POTCAR file out of the folder with the 2.40 bohr cutoff radius. This is the exact LDA-1/2 corrected pseudopotential that can be used in large supercells involving rutile TiO_2.

8. In shDFT-1/2 calculations, you may scan either the inner cutoff radius, or the outer cutoff radius. In each case, you need to fix the other cutoff radius. Hence, it may take two or three rounds before you confirm the final optimal set of cutoff radii.