

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

---- For VASP

1. Visit <http://www.eedevise.com/dft-half/>



2. Select DFT-1/2 input settings as shown below. We use LDA-1/2 calculation for rutile  $\text{TiO}_2$  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.

<i>Only select the anion element.</i>			LDA(GGA)-1/2 program for VASP		
Element: <input type="text" value="O"/>	Strip - <input type="text" value="0.50"/> e	Power index <input type="text" value="20"/>			
Scan cutoff radii from <input type="text" value="2.0"/> bohr to <input type="text" value="2.8"/> bohr			<a href="#">Using power index 20, this is a good range for O.</a>		
XC <input type="text" value="LDA (Ceperley-Alder)"/>					
Upload POTCAR file and start the run:					
<input type="button" value="选择文件"/> POTCAR		<input type="button" value="Upload"/>			
*You can upload a composite POTCAR file including several elements (e.g., Ti and O), but the program will only correct the specified element					
<a href="#">This POTCAR file on local computer contains Ti_sv and O pseudopotentials with the LDA flavor.</a>					
<a href="#">Click here to download the user manual ...</a>					

The uploaded POTCAR file contains Ti\_sv and O pseudopotentials:

**PAW Ti\_sv 26Sep2005**

**12.000000000000000**

... ..

**End of Dataset**

**PAW O 22Mar2012**

**6.000000000000000**

... ..

**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.

Upload POTCAR file and start the run:

没有选择文件

*\*You can upload a composite POTCAR file including several elements (e.g., Ti and O), but the program will only correct the specified element*

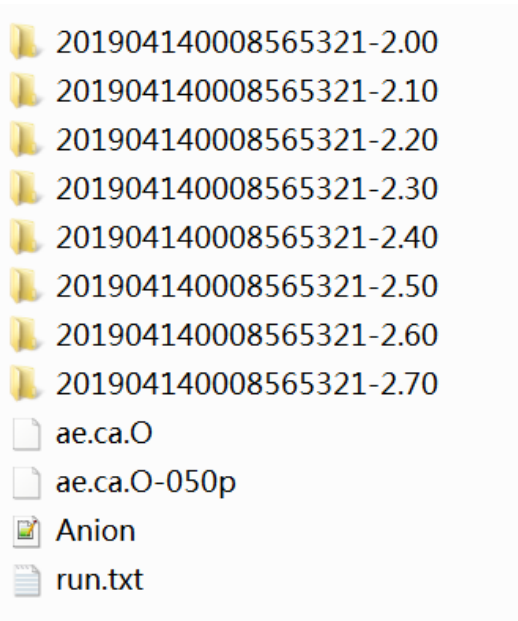
---

Processed with self-energy potential: O-050p.

Download zipped file at: <http://www.eedevise.com/pub-pot/201904140008565321.zip>

[Click here to download the user manual ...](#)

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<sub>2</sub>.
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.