Hands-On: FukuiGrid - Fukui Potential via SCPC

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1 Preparing the Input Files

Before executing the code, ensure that you have the required input files in the working directory. You should have the following CHGCAR files:

- CHGCAR file for the charge density of the neutral slab.
- CHGCAR file for the Fukui function.
- Planar average file of the SCPC correction potential.

The calculation of the charged system have be performed using the neutral pristine system as a reference.

2 Example: $v_{f^+}(r)$ of Rutile TiO_2 (110) Surface

To run FukuiGrid, execute the following command in the terminal:

```
python FukuiGrid.py
```

Upon execution, the following main menu will be displayed:

```
***** Main Menu *****
1 — Fukui Function via Interpolation
2 — Fukui Potential via Electrodes
3 — Fukui Potential via SCPC
4 — Process Grid Data
5 — Perturbative Expansion
6 — Exit

Choose an option: 3
```

Select option 3 for Fukui Potential via SCPC:

```
You selected option 3: Fukui Potential via SCPC

31 — Electrophilic Fukui function v_f-(r).
32 — Nucleophilic Fukui function v_f+(r).

Choose an option: 32
Name CHGCAR file of charge density of the neutral slab.
Enter file name: CHGCAR_00

Name CHGCAR file of Fukui function.
Enter file name: CHGCAR

Name SCPC correcton file.
Enter file name: z-vcor.dat
```

Once the calculation is complete, the output file “FUKUI.LOCPOT” will be generated. This file contains the computed Fukui potential mapped onto the original charge density grid.

After execution, you will return to the main menu. To exit FukuiGrid, choose option 6:

```
Choose an option: 6
You selected option 6: Goodbye!
```

In addition to the Fukui potential grid file, the code automatically generates a plot of the planar averages of the corrected and uncorrected potentials, as shown in Fig. 1.

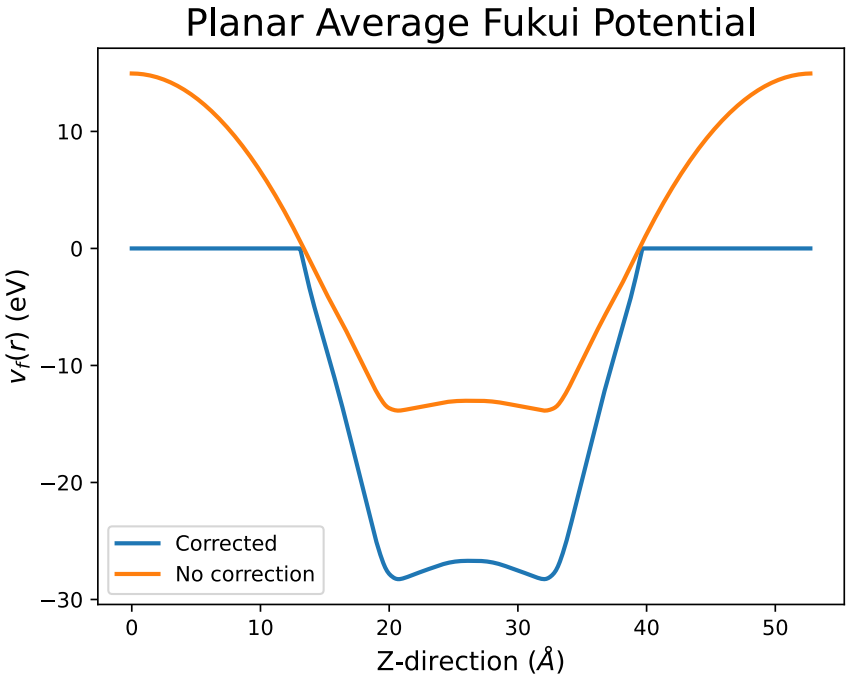

Figure 1: Planar average of Fukui potentials.