Hands-On: FukuiGrid - Fukui Potential via Electrodes

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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.

1.1 Obtaining the Dielectric Constant

The dielectric constant of a material is an essential parameter for the calculation of the Fukui potential via electrodes. This value can be obtained from experimental measurements or computed using Density Functional Perturbation Theory (DFPT) within VASP. The dielectric constant is calculated in a bulk calculation by setting the following flag in the INCAR file:

```
LEPSILON = .TRUE.
```

By default, 'LEPSILON' is set to '.FALSE.'. When 'LEPSILON = .TRUE.', VASP determines the static dielectric matrix, the ion-clamped piezoelectric tensor, and the Born effective charges. This calculation must be performed for the bulk system before proceeding with the FukuiGrid calculations.

The macroscopic dielectric constant can be computed using the following relations:

$$\text{VCDIEL} = \frac{\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}}{3} \tag{1}$$

$$\text{VCDIEL} = (\varepsilon_{xx} \cdot \varepsilon_{yy} \cdot \varepsilon_{zz})^{1/3} \tag{2}$$

where ε_{ij} are elements of the dielectric tensor.

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: 2
```

Select option 2 for Fukui Potential via Electrodes:

```
You selected option 2: Fukui Potential via Electrodes' method

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

Dielectric constant value.
Value: 7.34
```

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.

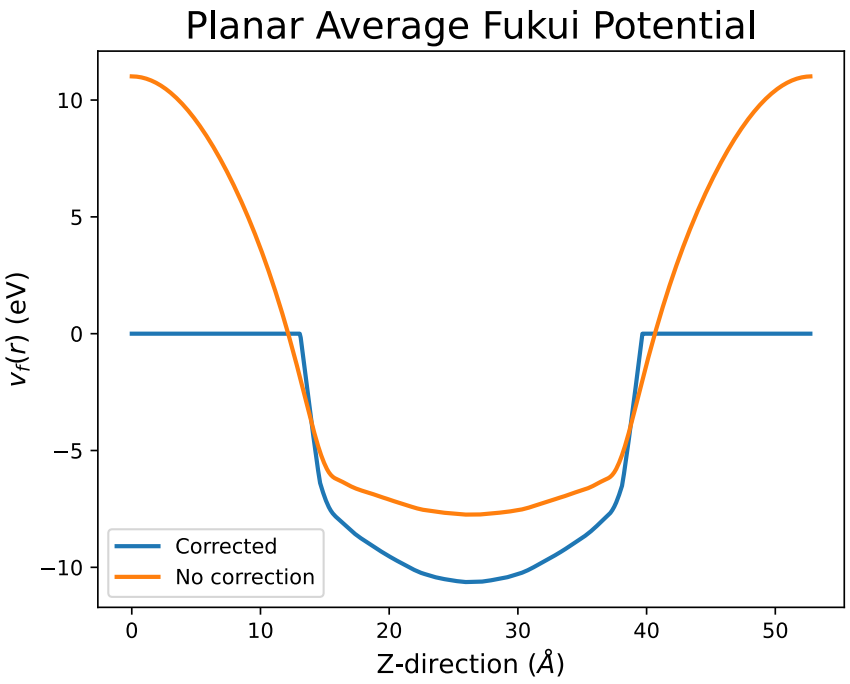

Figure 1: Planar average of Fukui potentials.