Hands-On: FukuiGrid - Fukui Functions $f^+(r)$ by Interpolation

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1 Running FukuiGrid

Before executing the code, ensure that you have the required input files in the working directory. You should have four CHGCAR files corresponding to the system at different charge states:

- CHGCAR for the neutral system ($\delta N = 0.0$).
- CHGCAR files for the system with fraction charges ($\delta N = +0.05, +0.10, +0.15$).

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: 1
```

Select option 1 for Fukui Function via Interpolation:

```
Chose option 1: Fukui Function via Interpolation.

11 Electrophilic Fukui function f⁻(r).
12 Nucleophilic Fukui function f⁺(r).
Choose an option: 12
```

If you select option 12, you will be prompted to enter the CHGCAR files:

```
Name CHGCAR files with δN: 0.0, +0.05, +.010 and +0.15
Enter name of file 1:
```

Once the calculation is complete, the output file "CHGCAR_FUKUI.vasp" will be generated. This file contains the computed Fukui function 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!
```

2 Example: ZrC (001) Surface

For the files available at `https://github.com/cacarden/FukuiGrid/tree/main/examples/Interpolation/fukui+`, which correspond to the ZrC (001) surface, the computed Fukui function $f^+(r)$ is obtained and is shown in Fig. 1.

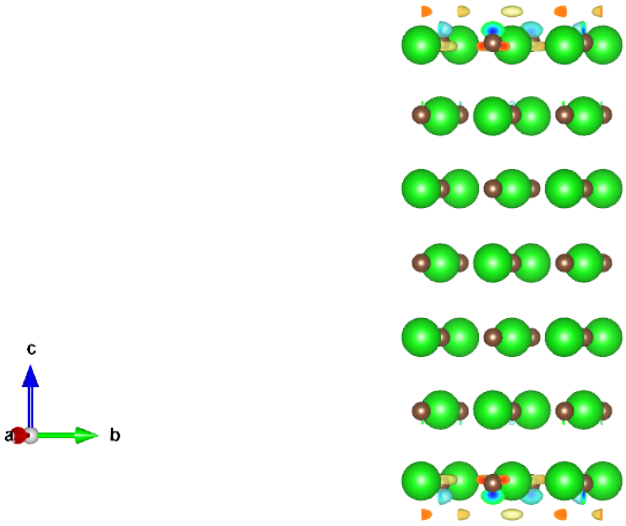

Figure 1: Isosurface representation of $f^+(r)$ with isovalue 0.0015 a_0^{-3}.