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

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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 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 ($\delta N = -0.05, -0.10, -0.15$).

2 Example: TiC (001) 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: 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: 11
```

If you select option 11, you will be prompted to enter the CHGCAR files:

```
Name CHGCAR files with δN: −0.15, −0.10, −0.05, and 0.0
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.

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

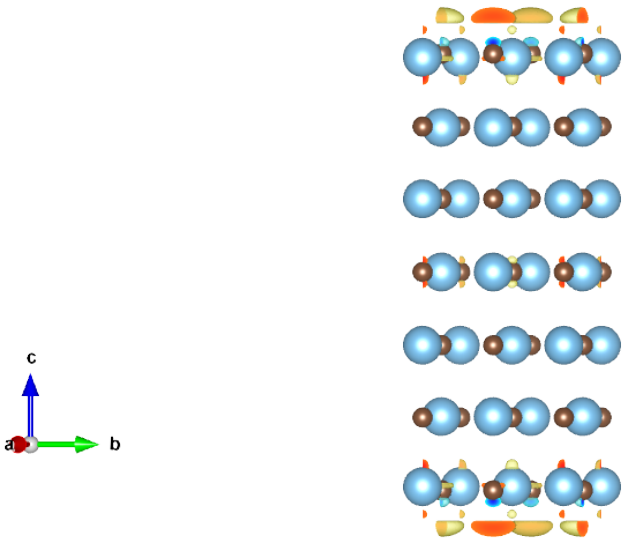

Figure 1: Isosurface representation of $f^{-}(r)$ with isovalue 0.002 a_0^{-3}.