Hands-On: FukuiGrid - Perturbative expansion

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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 files:

- Electrostatic potential file of the neutral system.
- Fukui potential file.
- Charge density file of the neutral slab (required for reactivity map).

2 Example: Interaction of Rutile TiO_2 (110) Surface with an electron-donor specie

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: 5
```

Select option 5 for Perturbative Expansion:

```
You selected Perturbative Expansion.
ΔU(r) = qΦ(r) − qΔNv_f±(r)

Name of LOCPOT file with Electrostatic potential Φ(r).
Enter name of LOCPOT: LOCPOT_00

Name of LOCPOT file with Fukui potential v_f±(r).
Enter name of LOCPOT: FUKUI.LOCPOT

Enter the change in the number of electrons ΔN:
ΔN: 0.2

Enter the charge q of active site:
q: −0.1

Do you want a heat map of ΔU(r)?
yes or no: yes
```

Once the calculation is complete, the output file "MODELPOT.LOCPOT" will be generated. This file contains the interaction energy of a point charge mapped onto the original potential 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 interaction energy grid file, the code automatically generates a plot of a heat map mapped onto the electron density isosurface ($\rho \approx 10^{-3}\, a_0^{-3}$), as shown in Fig. 1.

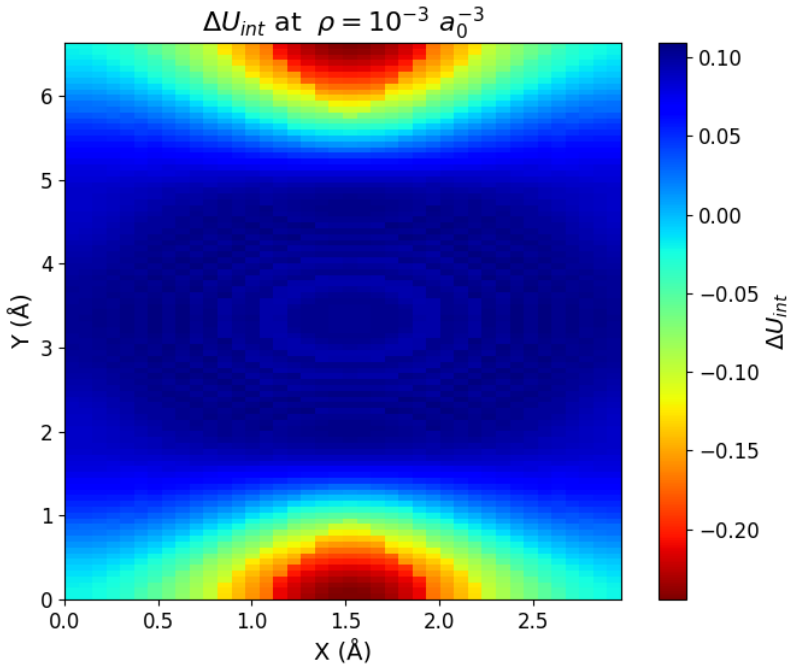

Figure 1: Heat map of the modelled interaction energy.