

Automated Fatband Generation in SIESTA

The Computational Physicist

Requirements

- **Utilities Required:**

- COOP/fat
- COOP/mprop
- Bands/eigfat2plot
- Bands/gnubands

- **Bash Scripts:**

- e_ef.sh
- eps_jpg.sh
- fatband.in
- fatband.sh

- **Libraries:**

- Gnuplot
- Python 3.0

- **Tags in input.fdf File:**

COOP.Write	true
WFS.Write.For.Bands	true
WFS.band.min	1
WFS.band.max	40

Initial Setup

1. **Install Required Libraries:** Ensure Gnuplot and Python 3.0 are installed.
2. **Set Up Executable Files and Scripts:**
 - Grant execute permissions to required files.
 - Copy executable files and scripts to /usr/local/bin for easy access.
3. **Optimize Structure:**
 - Include necessary tags in the input.fdf file for accurate fatband plotting.
4. **Edit fatband.in File:** Customize settings as needed for orbital and sub-orbital contributions.
5. **Execute fatband.sh:** Run the main script to automate fatband generation and produce plots.

Thank you !!!