Energy-Dia Demo Collection

This document introduces all features of the Energy-Dia library step by step. Starting from simple examples, it progresses to more complex chemically meaningful diagrams.

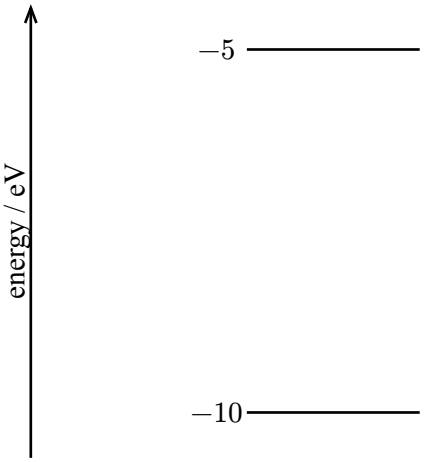
All diagrams can adjust size using `width` and `height` parameters.

Note: The energy values used in the examples were generated by an LLM or adjusted for visual appeal, so their scientific accuracy is not guaranteed. Please be aware of this.

1. Basics of Atomic Orbital Diagrams

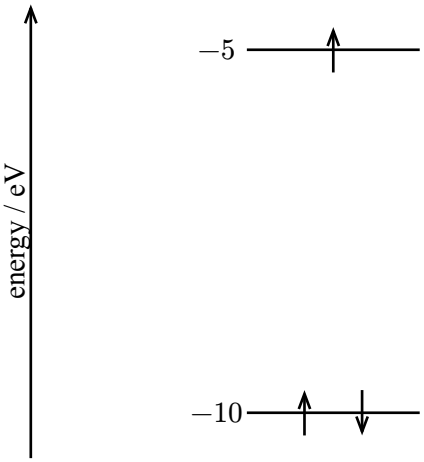
1.1 Simplest Example

A minimal example showing only energy levels.



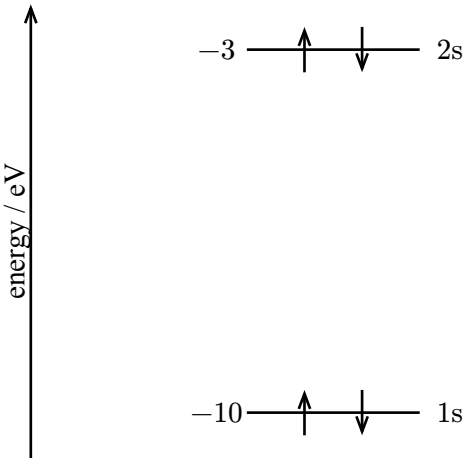
1.2 Basic Example with Electrons

Energy levels containing electrons. Electrons are automatically placed.



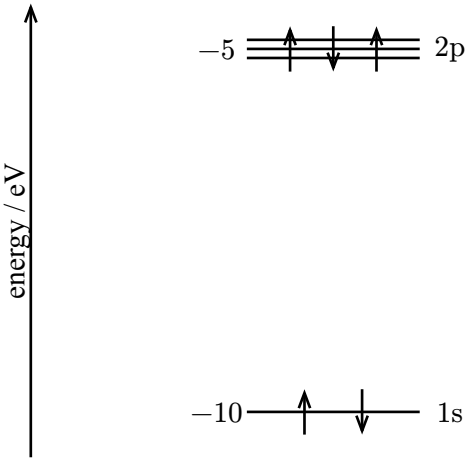
1.3 With Captions

Display orbital names as captions.



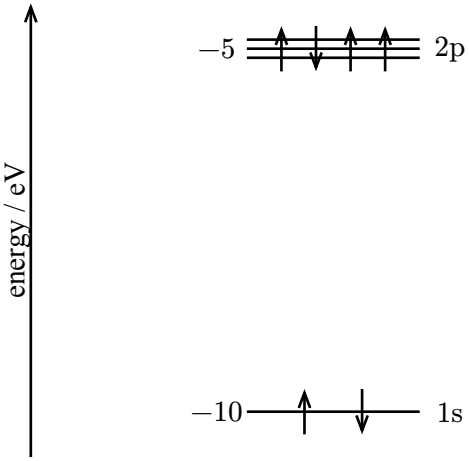
1.4 Representing Degenerate Orbitals

Use degeneracy to represent multiple orbitals at the same energy level.



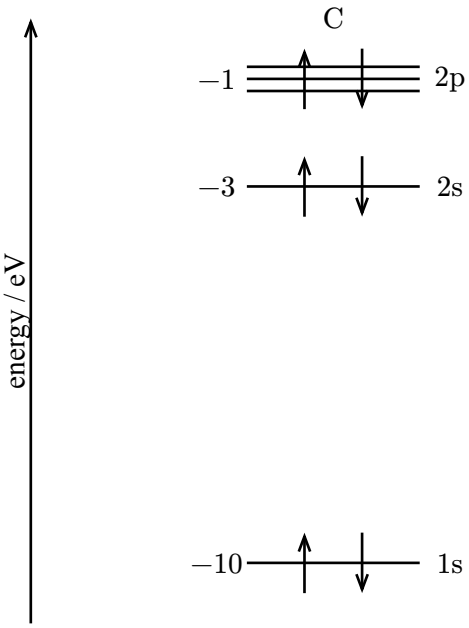
1.5 Specifying Spin-Up Electrons

You can explicitly specify the number of spin-up electrons with the `up` parameter. If not specified, they are placed alternately automatically.



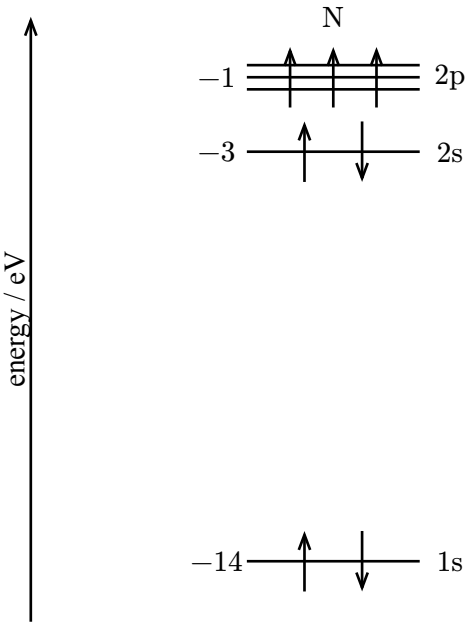
1.6 Displaying Atomic Name

You can display the atomic name with the `name` parameter.



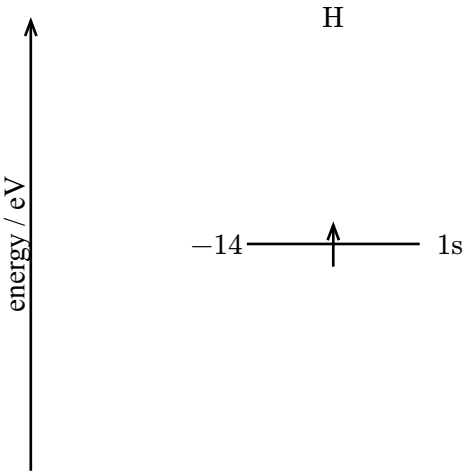
1.7 Hiding Energy Values

You can hide energy value labels with `exclude_energy: true`.

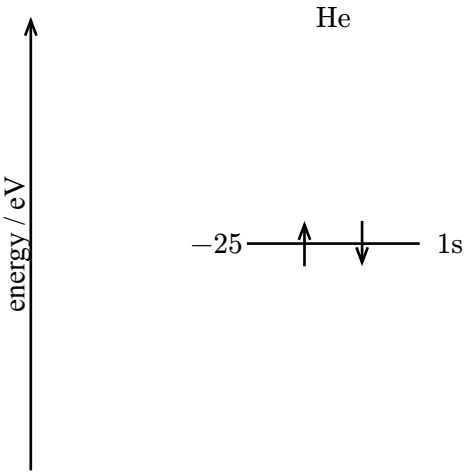


2. Electron Configurations of Real Atoms

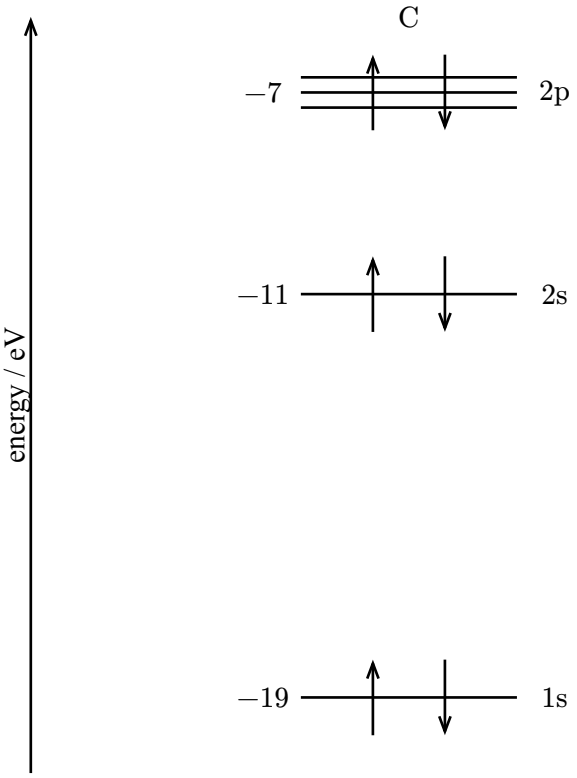
2.1 Hydrogen (H)



2.2 Helium (He)

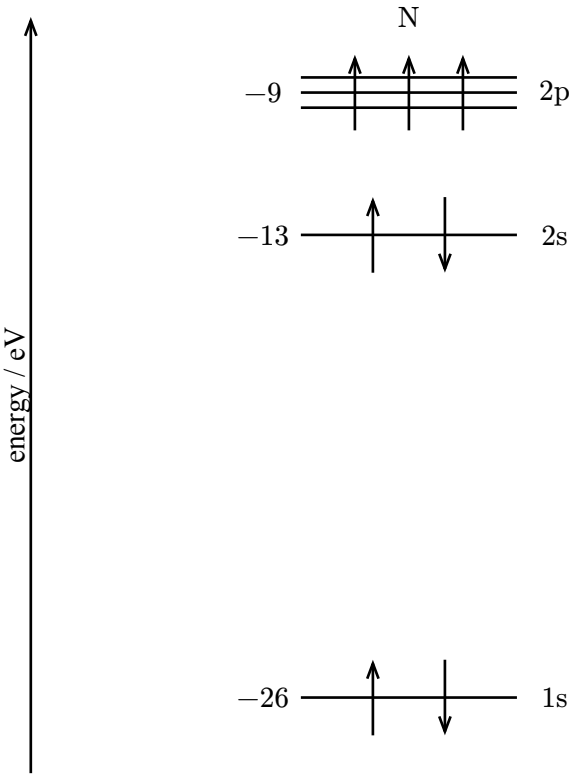


2.3 Carbon (C)

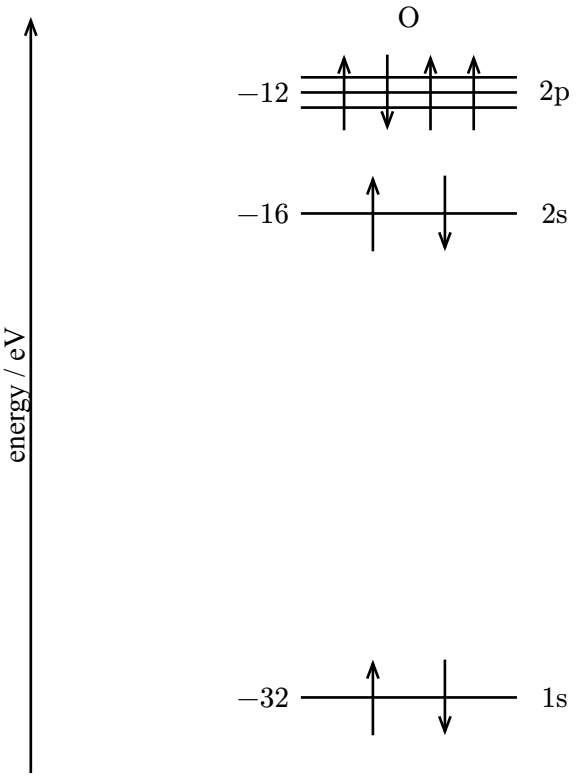


2.4 Nitrogen (N)

Electron configuration following Hund's rule (in degenerate orbitals, electrons occupy separate orbitals).



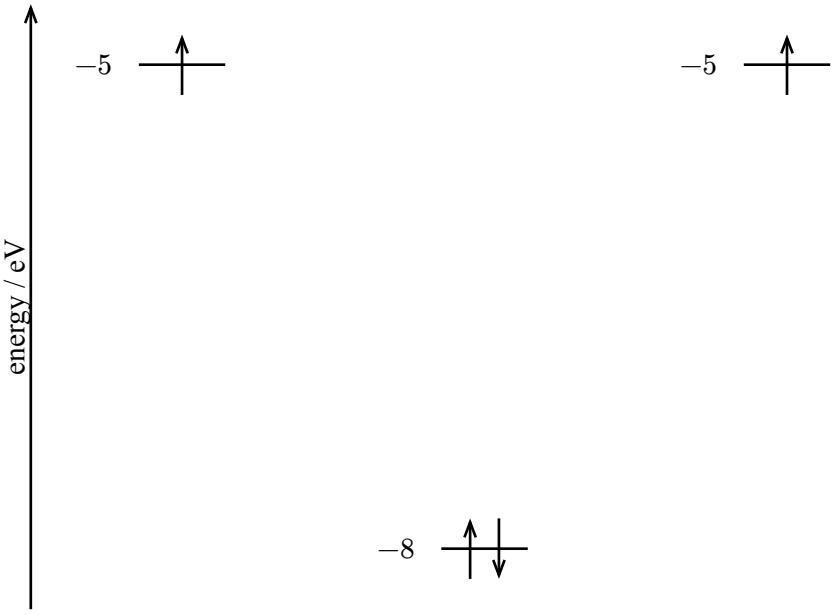
2.5 Oxygen (O)



3. Basics of Molecular Orbital Diagrams

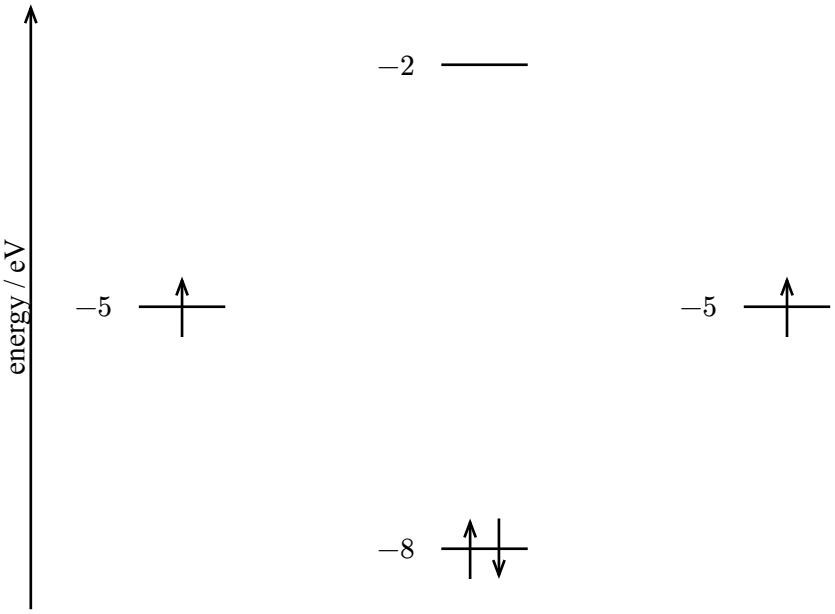
3.1 Simplest MO Diagram

A minimal example where one molecular orbital is formed from two atomic orbitals.



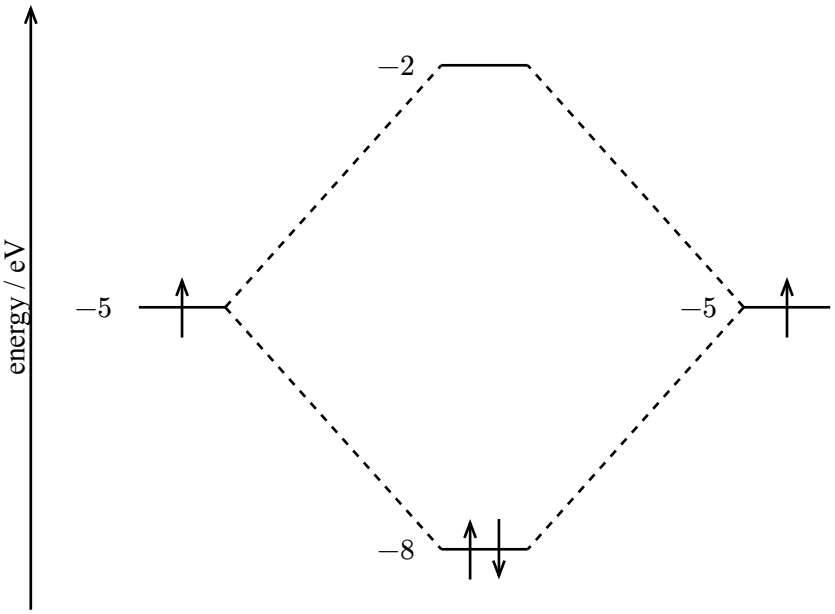
3.2 Bonding and Antibonding Orbitals

Display both bonding and antibonding orbitals.



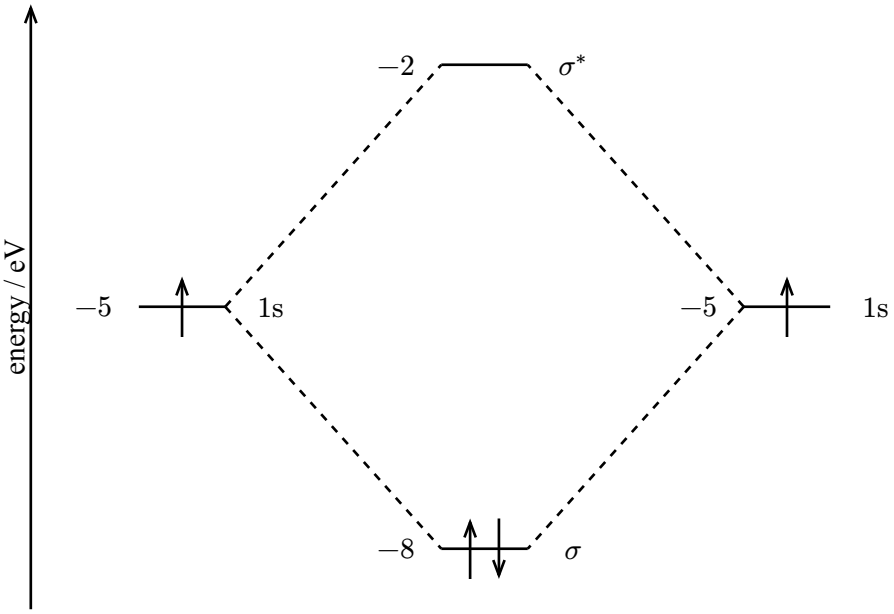
3.3 Connections Between Orbitals

Use labels to show correspondence between atomic and molecular orbitals.



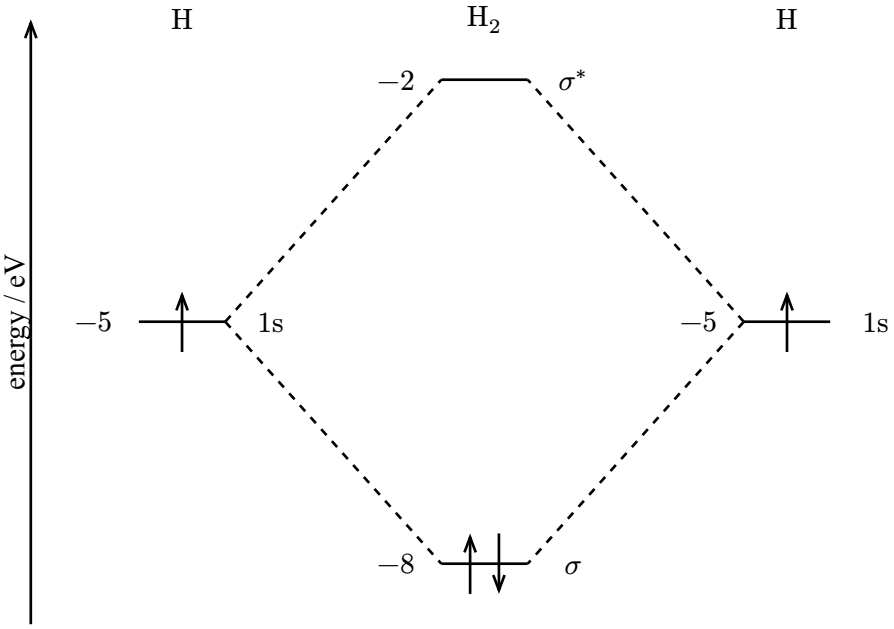
3.4 With Captions

Add captions to orbitals.



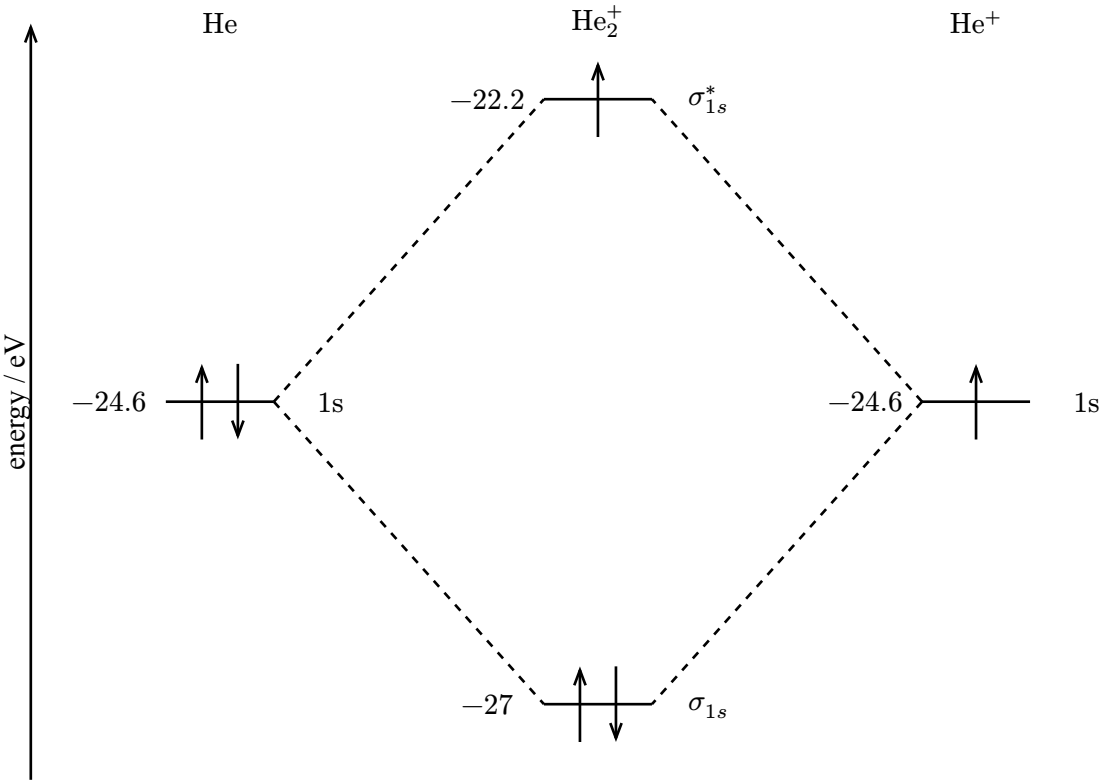
3.5 Displaying Atomic and Molecular Names

Display names for left atom, central molecule, and right atom with the `names` parameter.

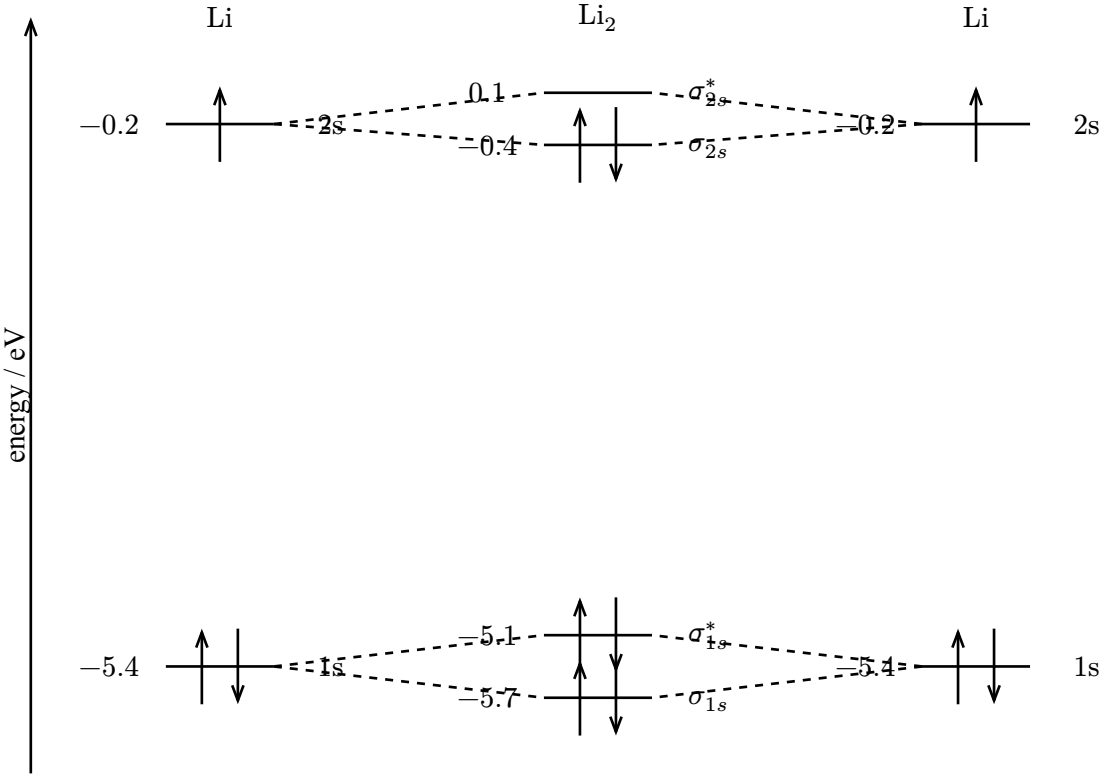


4. MO Diagrams of Real Molecules

4.1 Helium Molecular Ion (He_2^+)

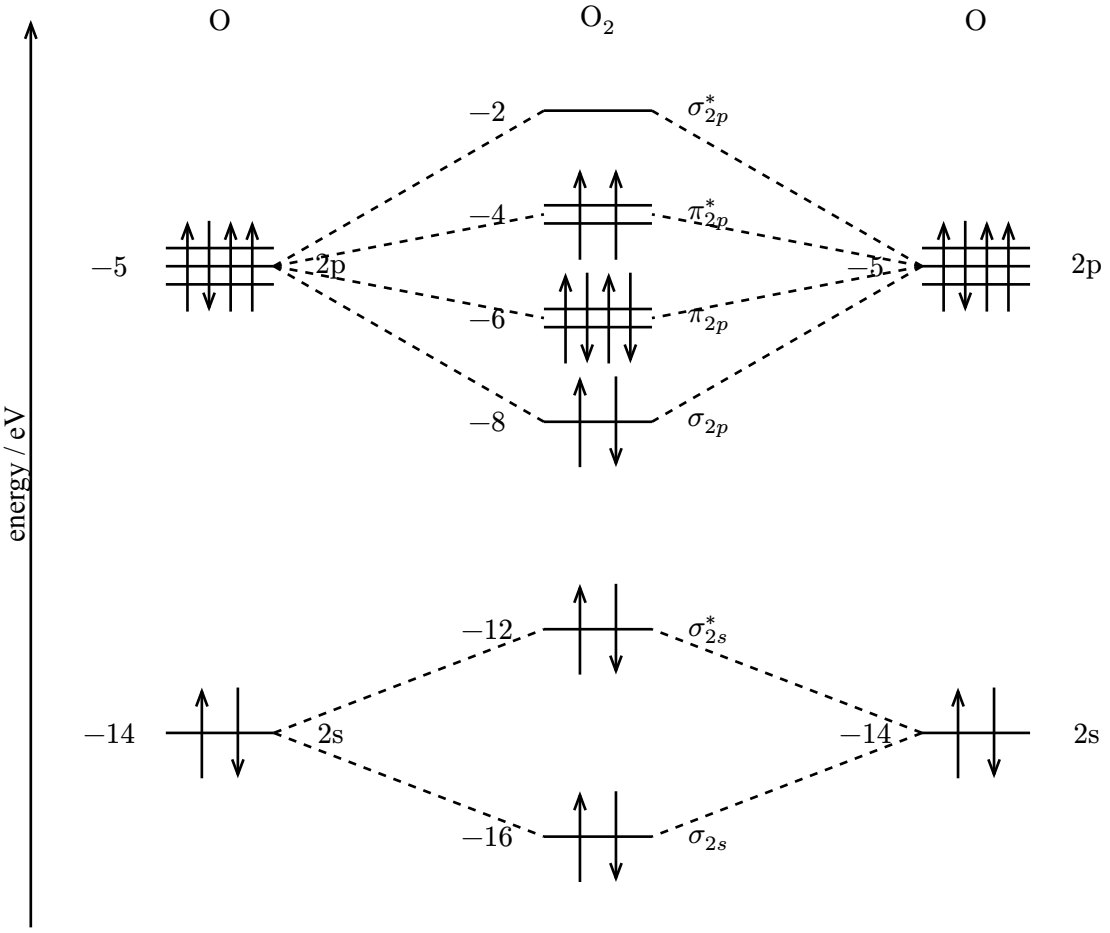


4.2 Lithium Molecule (Li_2)

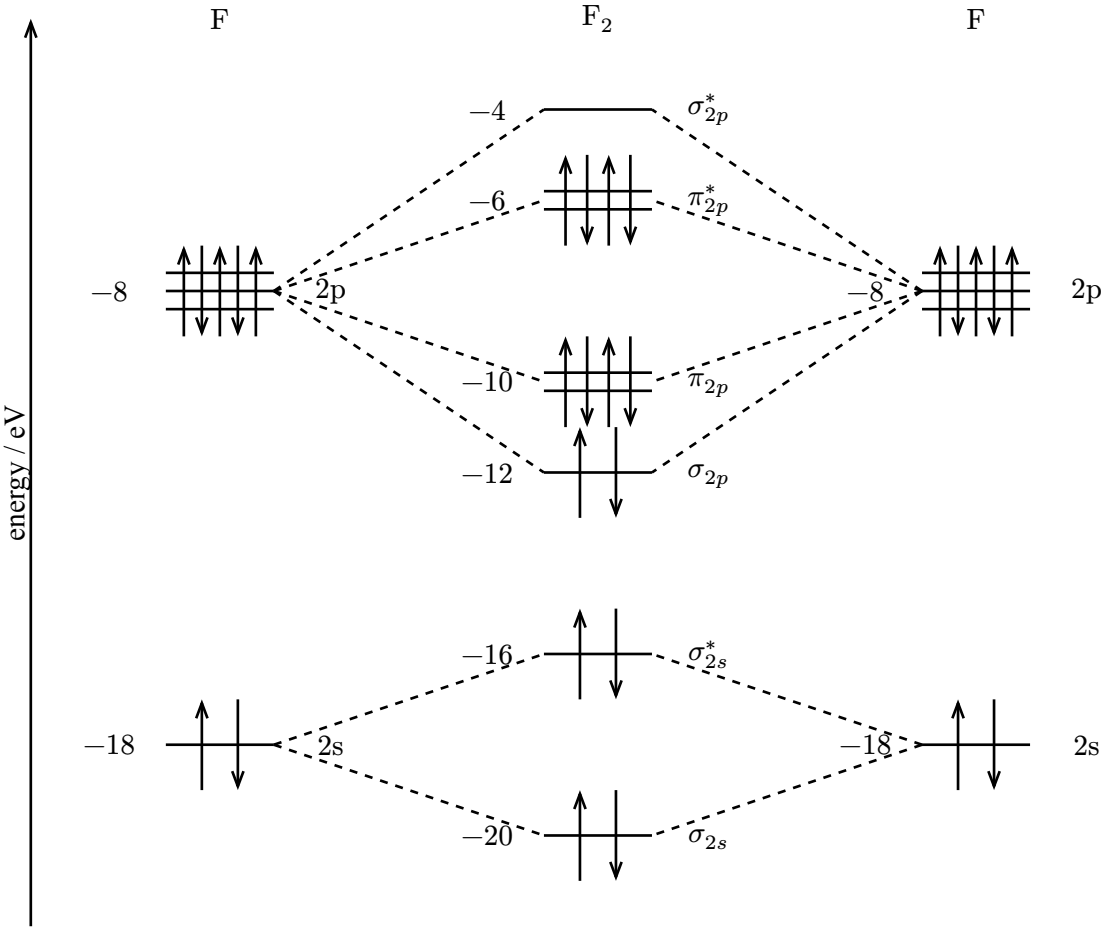


4.3 Oxygen Molecule (O_2)

A molecule with a double bond that exhibits paramagnetism. This is the complete example introduced in the README.



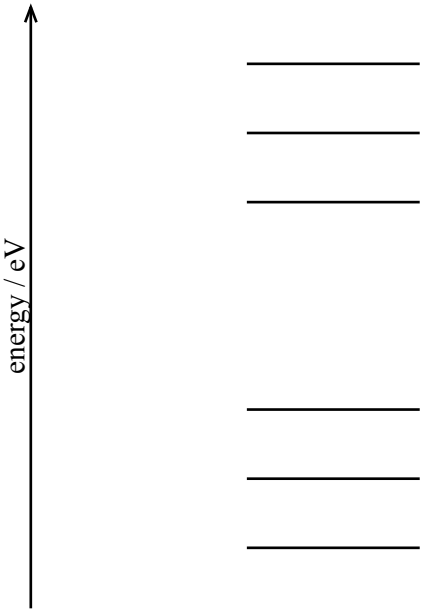
4.4 Fluorine Molecule (F_2)



5. Band Structure Diagrams

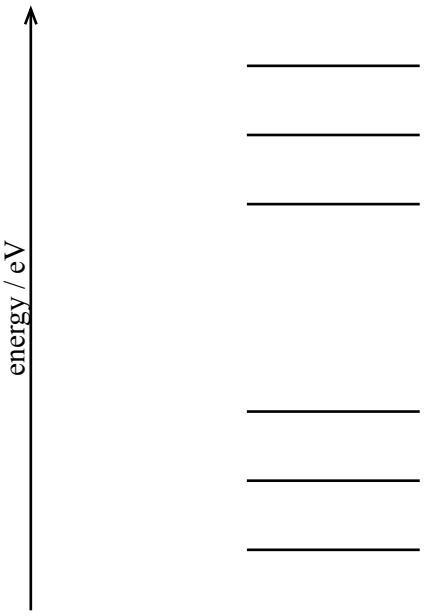
5.1 Basic Band Structure

Display manually entered energy levels.



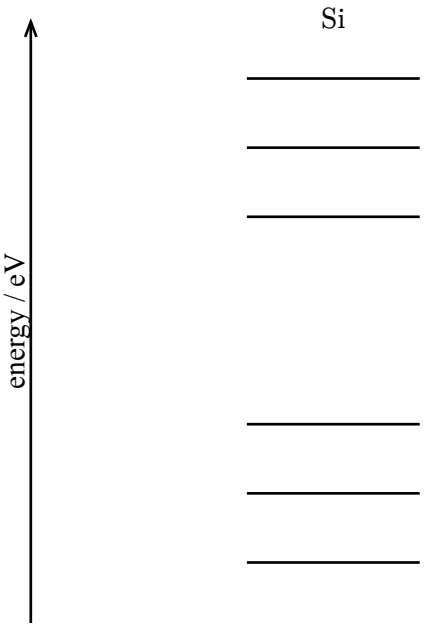
5.2 With Energy Labels

Display energy values with `include_energy_labels: true`.



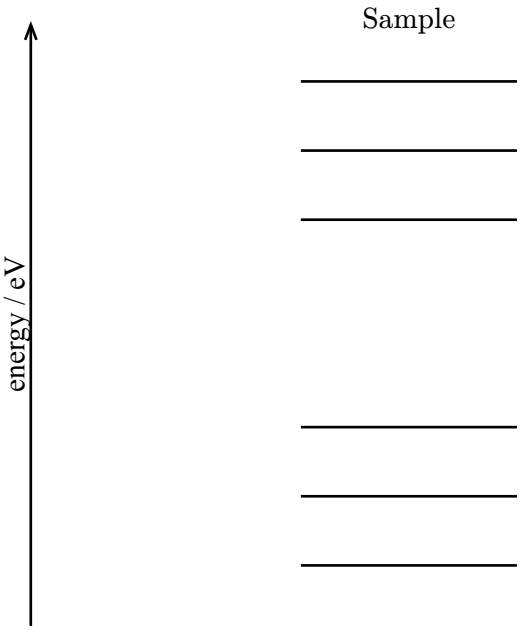
5.3 With Material Name

Display material name with the `name` parameter.



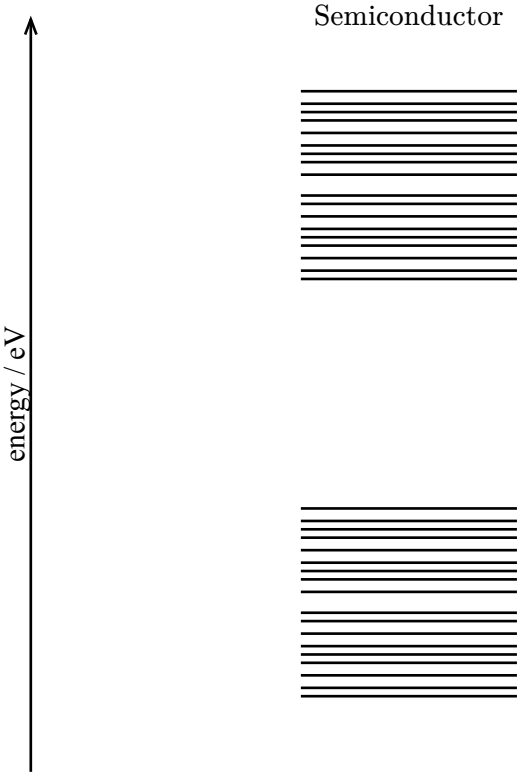
5.4 Loading from CSV Data

Load energy levels from a CSV file and display them.



5.5 Many Energy Levels

Band structures usually have many energy levels.



Summary

This demo introduced the following features:

Atomic Orbital Diagrams (AO):

- Basic energy level display
- Electron configuration
- Degenerate orbitals (degeneracy)
- Spin states (up parameter)

- Atomic name display
- Show/hide energy values

Molecular Orbital Diagrams (MO):
- Transition from atomic orbitals to molecular orbitals
- Connections between orbitals
- Degenerate molecular orbitals
- Display of atomic and molecular names
- Electron configurations of real molecules

Band Structure Diagrams (Band):
- Basic band display
- Loading data from CSV
- Show/hide energy labels
- Display of many energy levels

For detailed parameter descriptions, please refer to README.md.