

# 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.

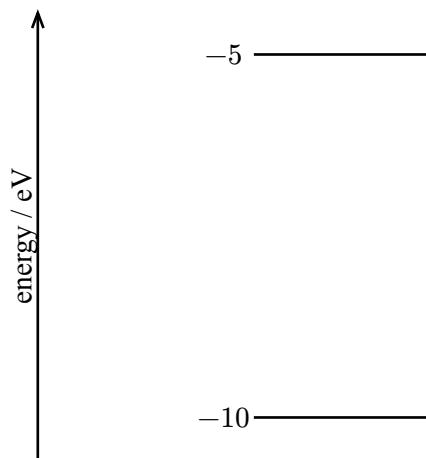
All diagrams can adjust size using width and height parameters.

**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

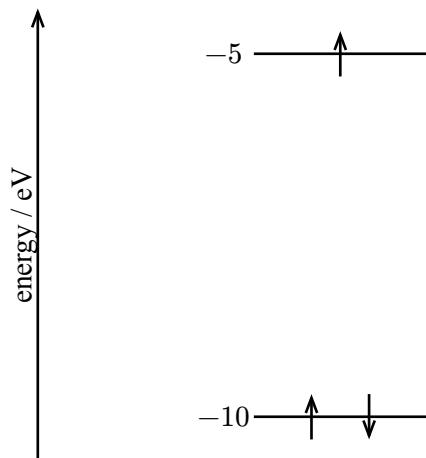
### 1.1 Simplest Example

A minimal example showing only energy levels.



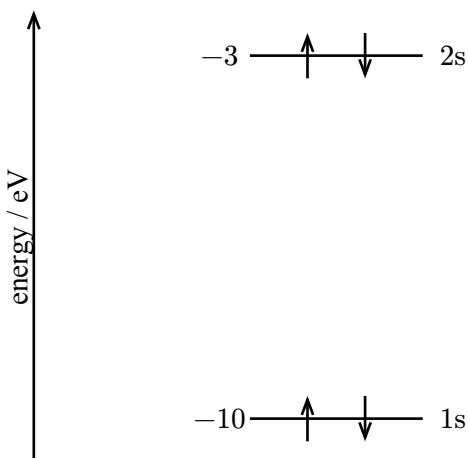
### 1.2 Basic Example with Electrons

Energy levels containing electrons. Electrons are automatically placed.



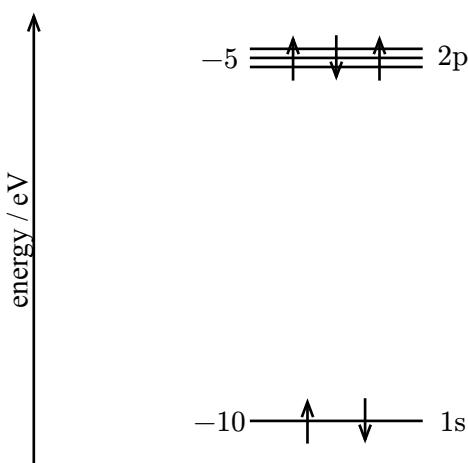
### 1.3 With Captions

Display orbital names as captions.



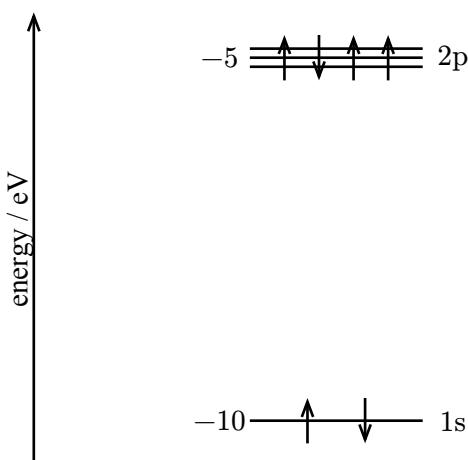
## 1.4 Representing Degenerate Orbitals

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



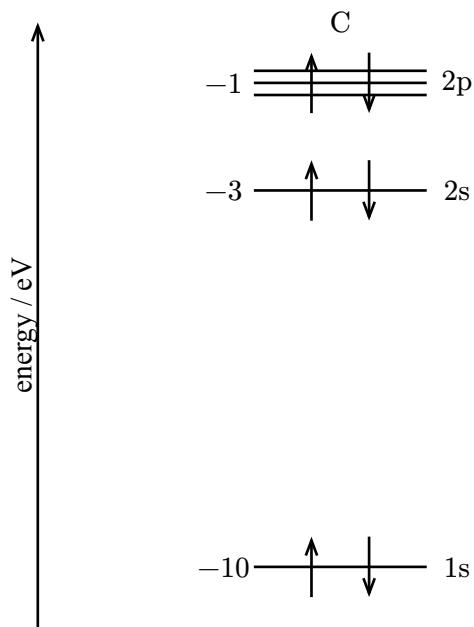
## 1.5 Specifying Spin-Up Electrons

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



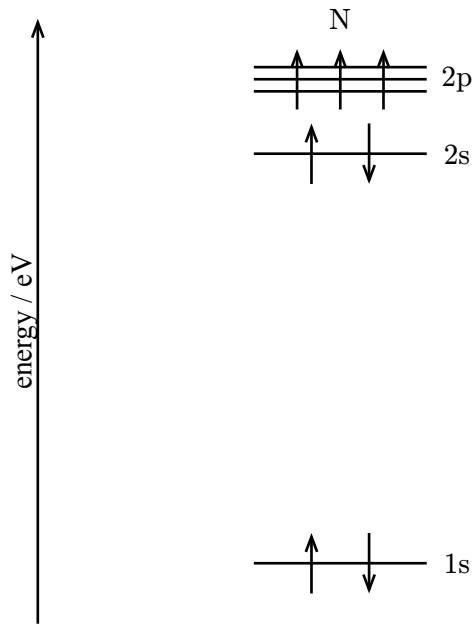
## 1.6 Displaying Atomic Name

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



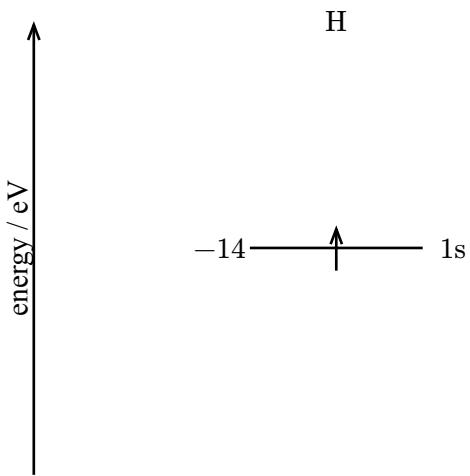
### 1.7 Hiding Energy Values

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

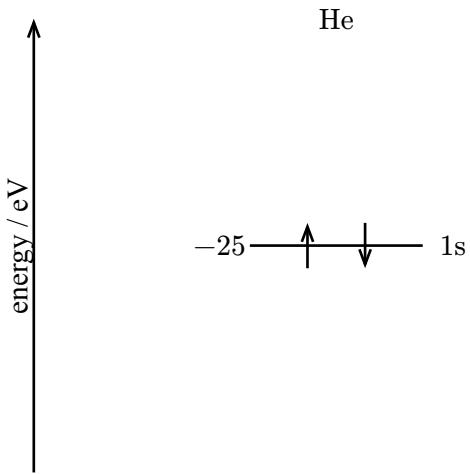


## 2. Electron Configurations of Real Atoms

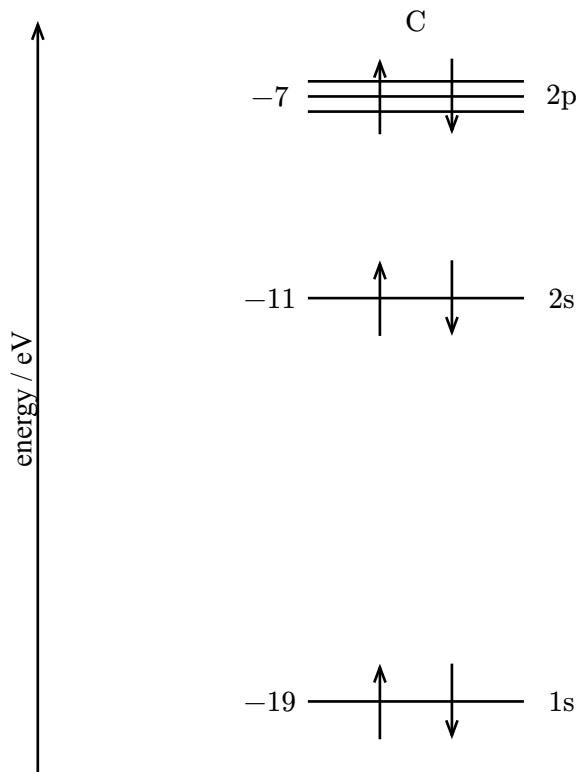
### 2.1 Hydrogen (H)



### 2.2 Helium (He)

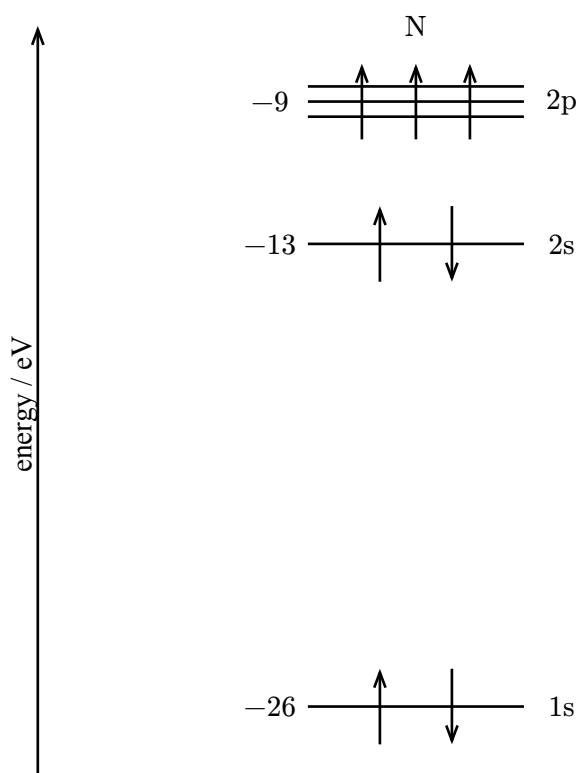


### 2.3 Carbon (C)

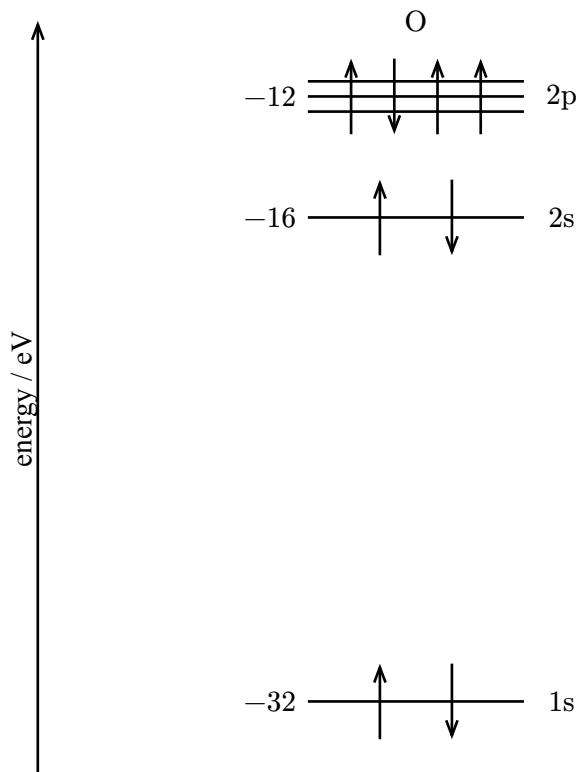


### 2.4 Nitrogen (N)

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



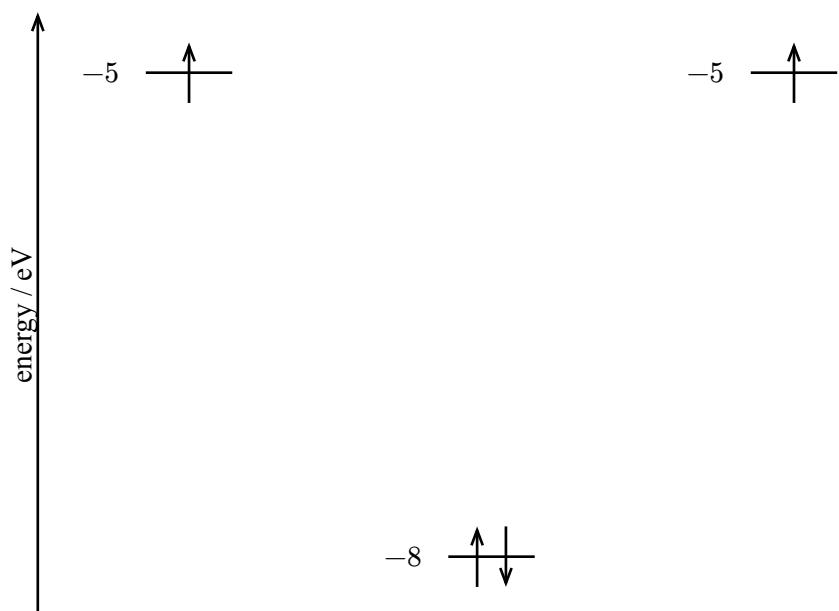
## 2.5 Oxygen (O)



## 3. Basics of Molecular Orbital Diagrams

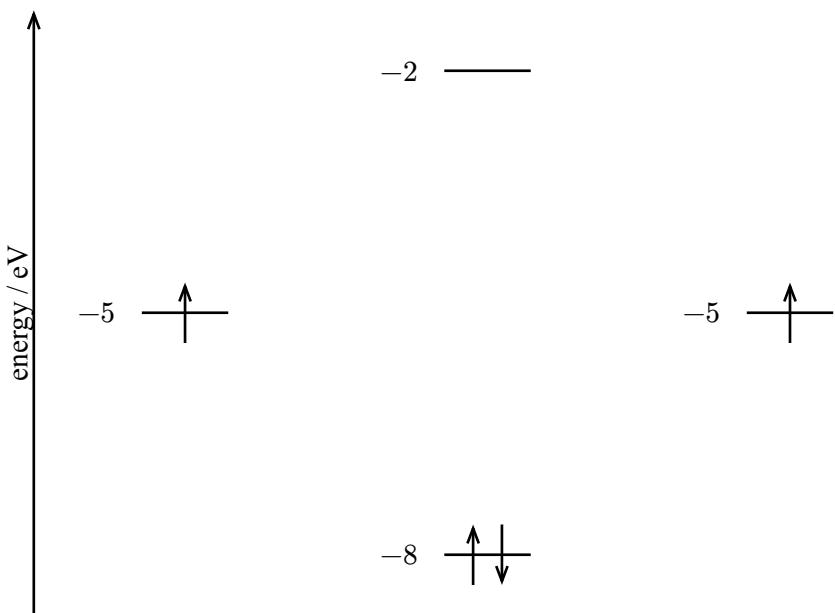
### 3.1 Simplest MO Diagram

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



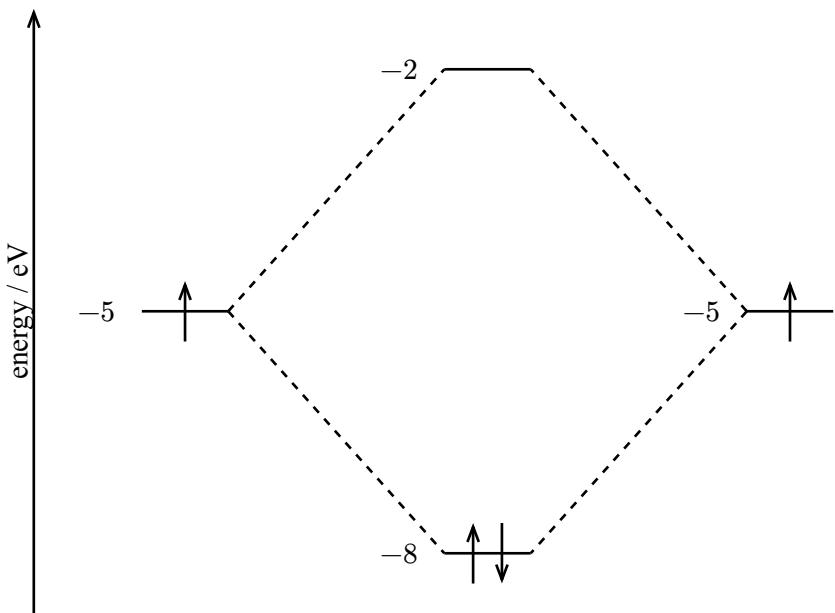
### 3.2 Bonding and Antibonding Orbitals

Display both bonding and antibonding orbitals.



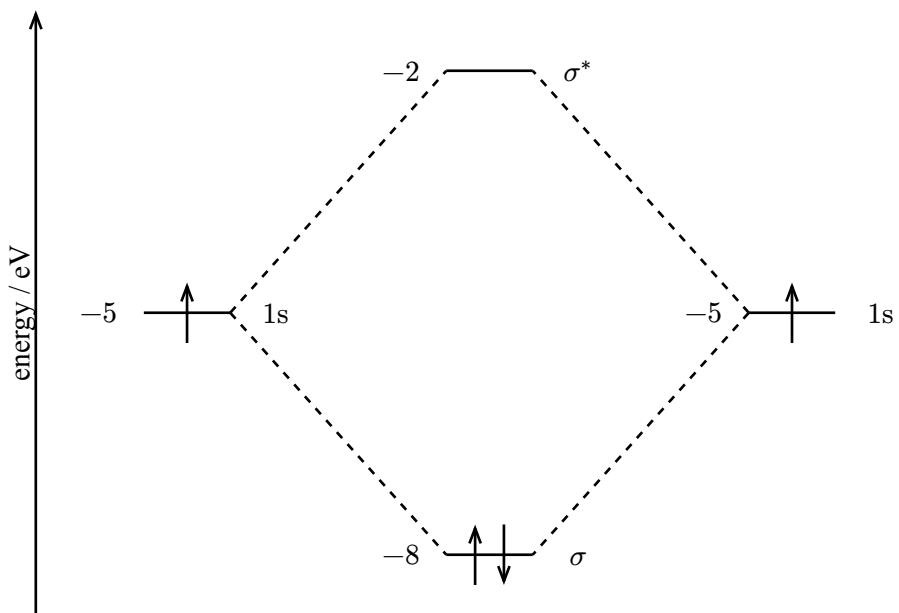
### 3.3 Connections Between Orbitals

Use labels to show correspondence between atomic and molecular orbitals.



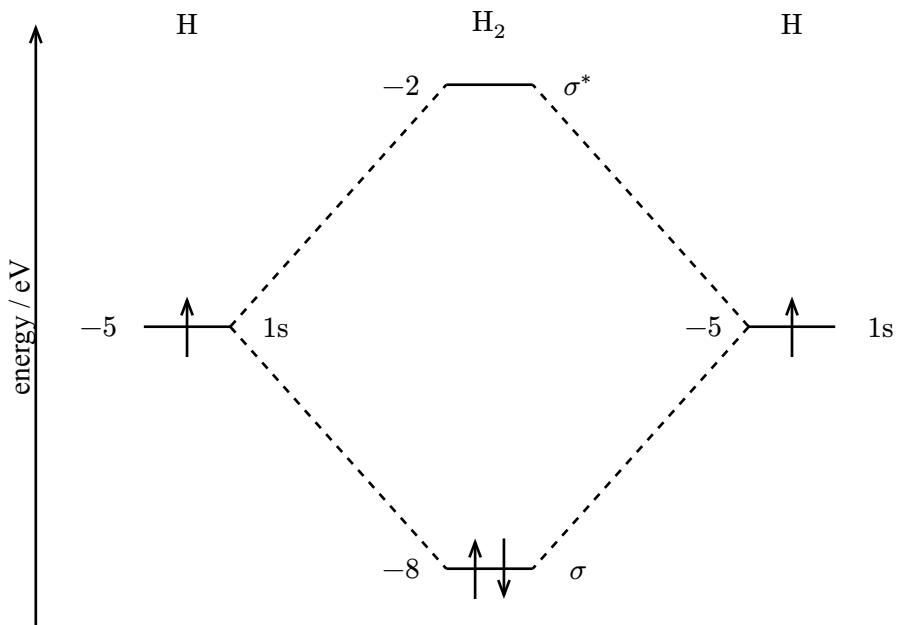
### 3.4 With Captions

Add captions to orbitals.



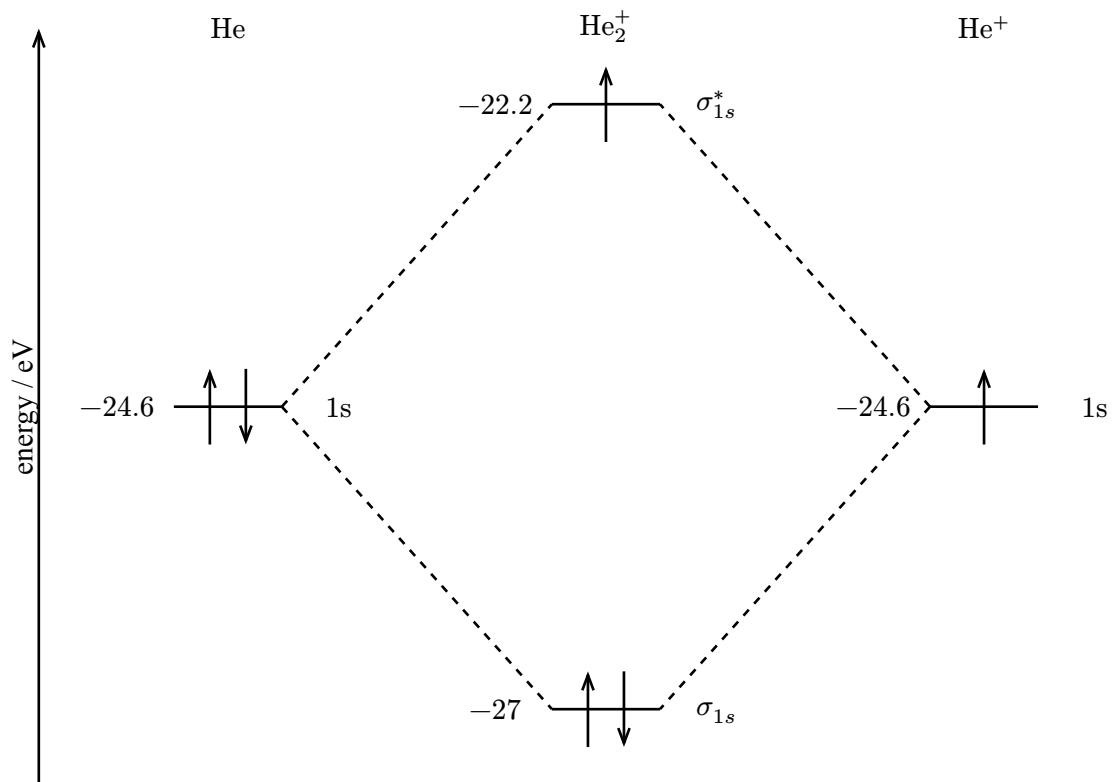
### 3.5 Displaying Atomic and Molecular Names

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

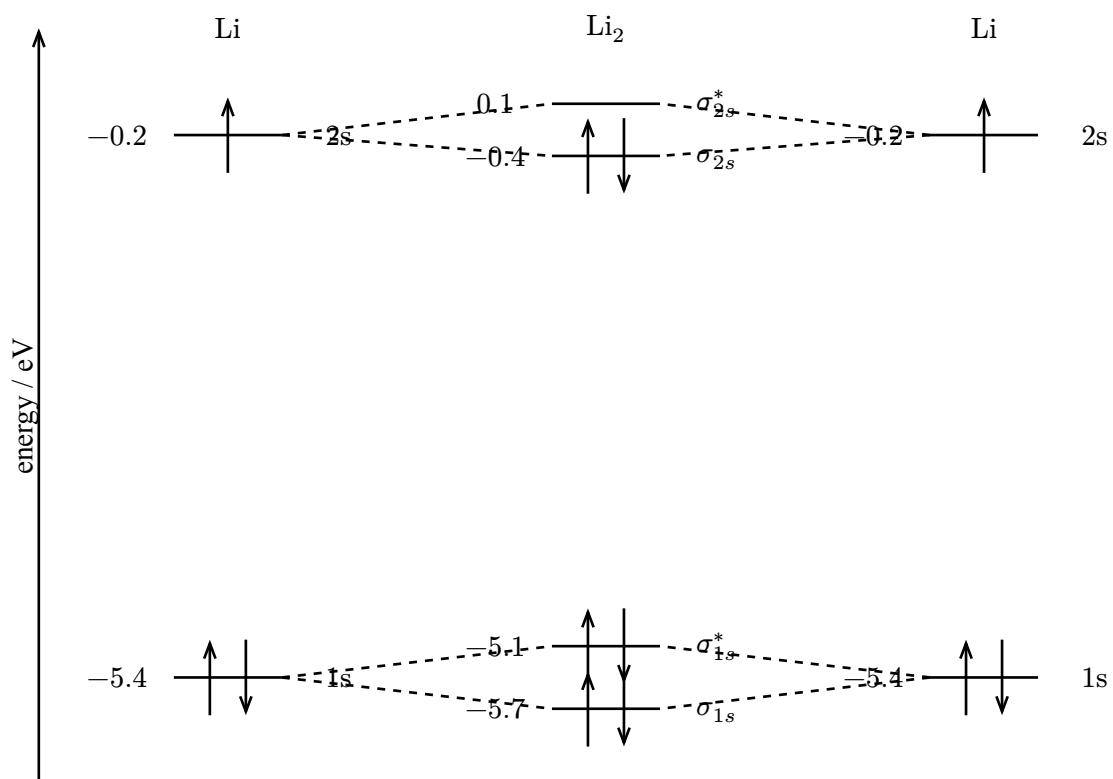


## 4. MO Diagrams of Real Molecules

### 4.1 Helium Molecular Ion ( $\text{He}_2^+$ )

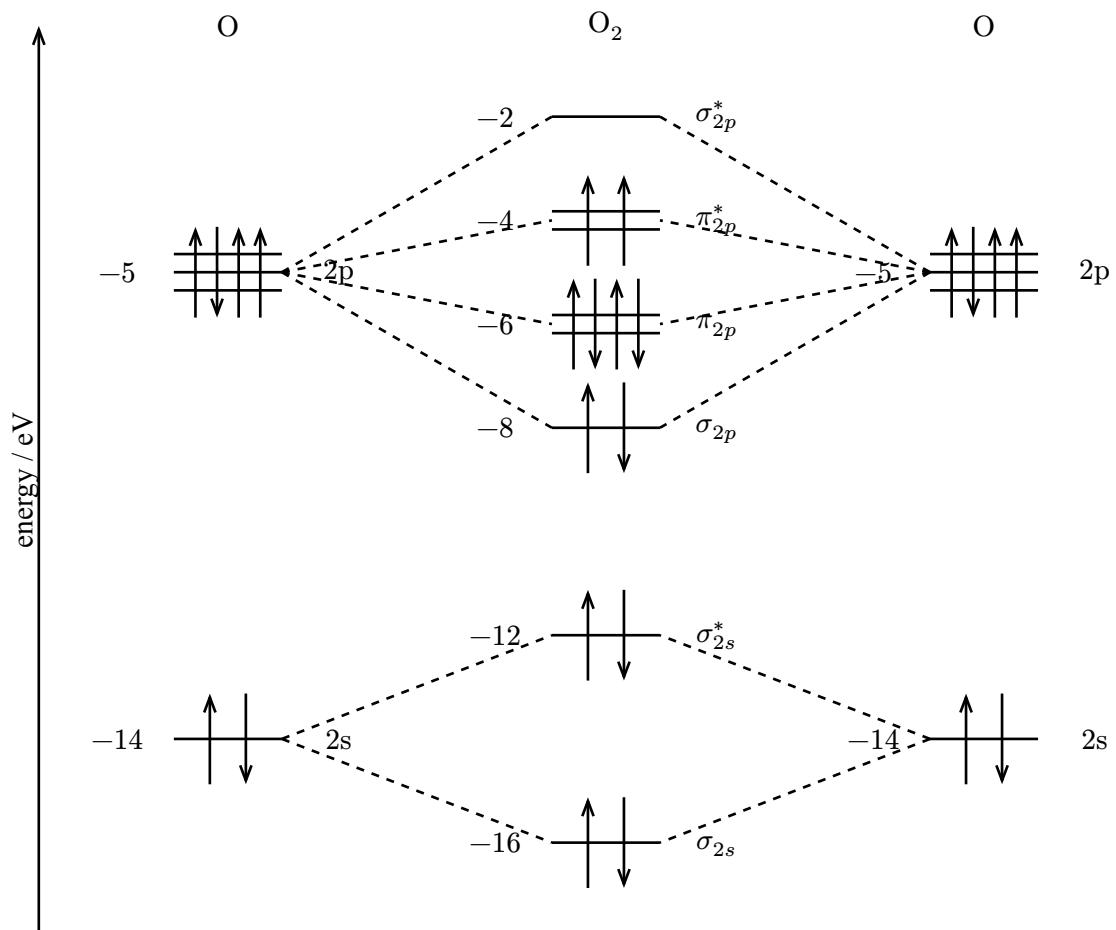


### 4.2 Lithium Molecule ( $\text{Li}_2$ )

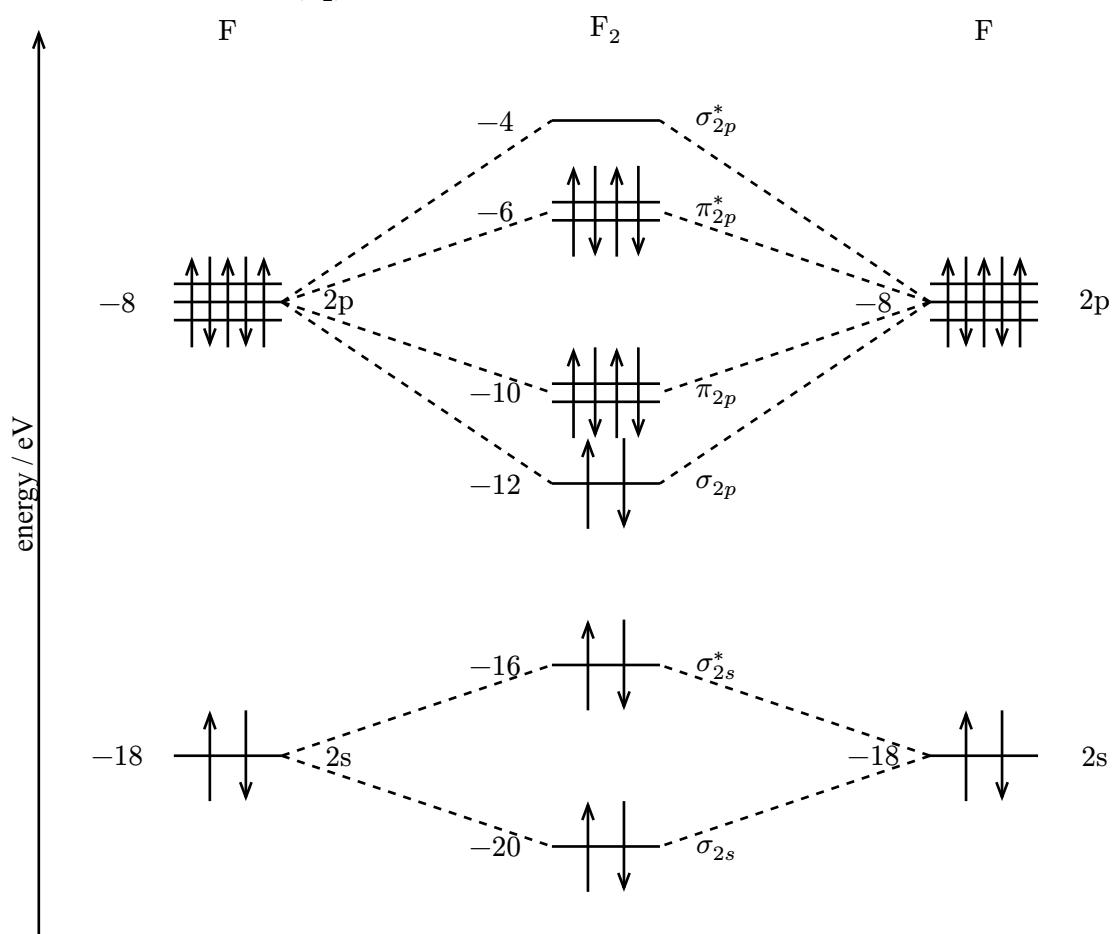


### 4.3 Oxygen Molecule ( $O_2$ )

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



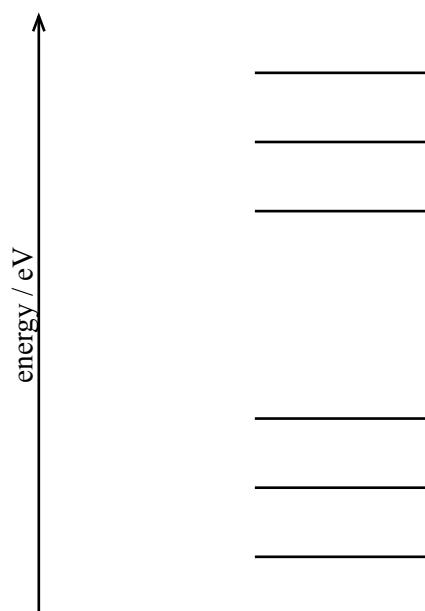
#### 4.4 Fluorine Molecule ( $F_2$ )



### 5. Band Structure Diagrams

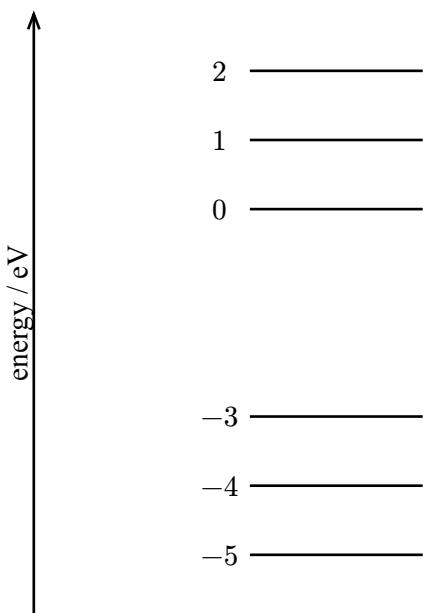
#### 5.1 Basic Band Structure

Display manually entered energy levels.



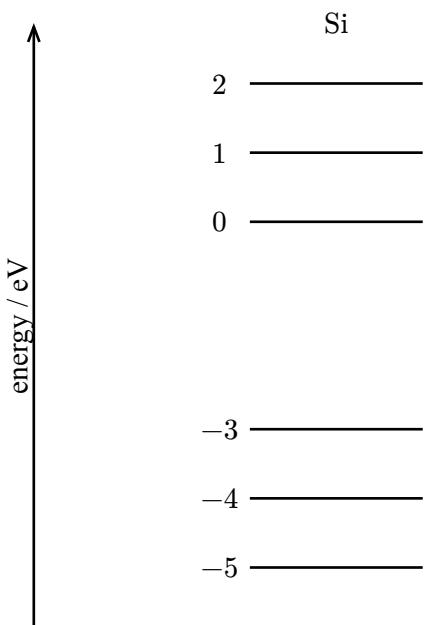
## 5.2 With Energy Labels

Display energy values with `include_energy_labels: true`.



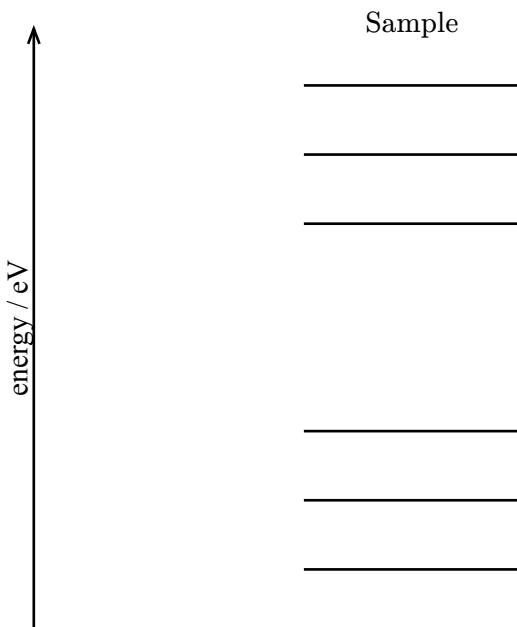
## 5.3 With Material Name

Display material name with the `name` parameter.



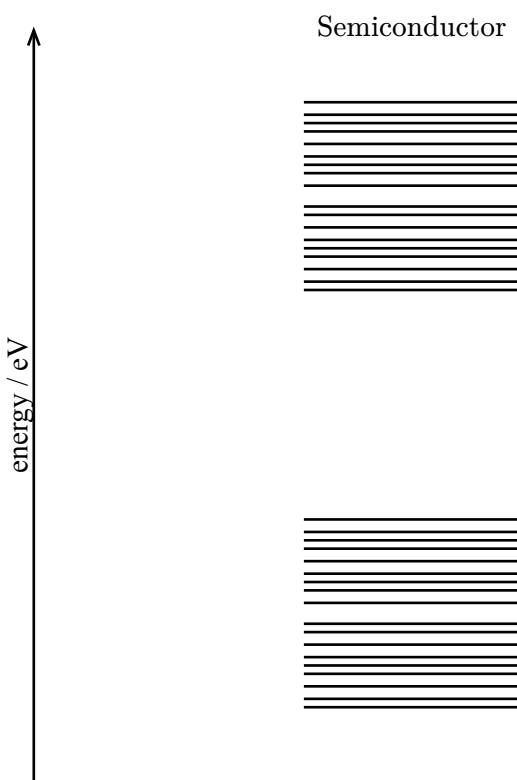
## 5.4 Loading from CSV Data

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.