1 Introduction

Energy-Dia is a Typst library for creating energy diagrams such as atomic orbital diagrams, molecular orbital diagrams, and band structure diagrams. It utilizes the CeTZ library to easily draw diagrams for chemistry and physics.

1.1 Features

- **Atomic Orbital Diagrams (AO)**: Visualize energy levels and electron configurations of atoms.
- **Molecular Orbital Diagrams (MO)**: Display molecular orbital formation and electron configurations.
- **Band Structure Diagrams**: Plot band structures.

1.2 Installation

To use this library, import as follows:

```
#import "@preview/energy-dia:0.1.0": *
```

2 API Documentation

The following sections document the functions provided by the Energy-Dia library.

- ao()
- band()
- mo()

2.0.1 ao

Display an energy level diagram for atomic orbitals

Arguments:

- width (length): Width of the diagram
- height (length): Height of the diagram
- levels (array of dictionaries): Energy level and electron count data. Each dictionary has the following keys:
  - energy (number): Energy value
  - electrons (number): Number of electrons (default: 0)
  - degeneracy (number): Degeneracy (default: 1)
  - caption (string): Caption (default: none)
  - up (boolean): Upward spin (default: none)

Example:

```
#ao(
  (energy: -1, electrons: 2),
  (energy: 0, electrons: 1)
)
```

2.0.1.1 Parameters

```
ao(
  width,
  height,
  ..levels
)
```

2.0.2 band

Display an energy level diagram for band structure

Arguments:

- width (length): Width of the diagram
- height (length): Height of the diagram
- include_energy_labels (boolean): Whether to display energy labels
- levels (array of numbers): List of energy level values

Example:

```
#band(
  -1, 0, 0.5, 1,
  include_energy_labels: true
)
```

2.0.2.1 Parameters

```
band(
  width,
  height,
  include_energy_labels,
  ..levels
)
```

2.0.3 mo

Display an energy level diagram for molecular orbitals

Arguments:

- width (length): Width of the diagram
- height (length): Height of the diagram
- atom1 (array of dictionaries): Energy level data for the left atom. Each dictionary has the following keys:
  - energy (number): Energy value
  - electrons (number): Number of electrons (default: 0)
  - degeneracy (number): Degeneracy (default: 1)
  - caption (string): Caption (default: none)
  - up (boolean): Upward spin (default: none)
- molecule (array of dictionaries): Energy level data for the molecule. Each dictionary has the following keys:
  - energy (number): Energy value
  - electrons (number): Number of electrons (default: 0)
  - degeneracy (number): Degeneracy (default: 1)
  - caption (string): Caption (default: none)
  - up (boolean): Upward spin (default: none)
- atom2 (array of dictionaries): Energy level data for the right atom. Each dictionary has the following keys:
  - energy (number): Energy value
  - electrons (number): Number of electrons (default: 0)
  - degeneracy (number): Degeneracy (default: 1)
  - caption (string): Caption (default: none)
  - up (boolean): Upward spin (default: none)
- connections (array): Connection data between orbitals

Example:

```
#mo(
  atom1: ((energy: -1, electrons: 2), (energy: 0, electrons: 1)),
  molecule: ((energy: -0.5, electrons: 2)),
```

```
  atom2: ((energy: -1, electrons: 2), (energy: 0, electrons: 1))
)
```

Warning: Each atom and molecular orbital is required to be an array. Therefore, even if there is only one orbital, do not forget to put a comma at the end.

2.0.3.1 Parameters

```
mo(
  width,
  height,
  atom1,
  molecule,
  atom2,
  ..connections
)
```

3 Examples

Please refer to demo/demo.typ for examples.