Adsorption Documentation

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Welcome to the documentation for the Adsorption script. This script facilitates the adsorption of molecules onto surfaces, offering the flexibility to manipulate both the adsorption position and the orientation of the molecule.

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1.1 Installation

To use the Adsorption script, follow these steps:

1. Install Python (if not already installed).
2. Install the Atomic Simulation Environment (ASE) library.
3. Make sure that tkinter package is installed for the GUI.
4. Download the Adsorption.py script from the provided source.
5. You're ready to use the script!

You can install the ASE library using pip: c .. code-block:: shell

    pip install ase

1.2 Usage

To use the Adsorption script, run it from the command line with the following syntax:

```
python3 Adsorption.py surface_file.vasp molecule_file.xyz --origine 0 --vertex 1 --
↪adsorb_index 2 --height 3.5 --theta_z 30
```

This command performs adsorption of a molecule on a surface. You need to provide the filenames of the surface and molecule files, as well as the indices of the atoms defining the direction of the molecule. Additionally, specify the index of the atom on the surface for adsorption, the desired adsorption height, and the angle of rotation arround z axis..

1.3 Examples

Here are some examples demonstrating the usage of the Adsorption script:

Example 1: Perform adsorption of a molecule on a surface

```
python3 Adsorption.py surface_file.vasp molecule_file.xyz --origine 0 --vertex 1 --
↪adsorb_index 2 --height 3.5 --theta_z 30
```

This example performs adsorption of a molecule on a surface using the specified input files and parameters.

1.4 Dependencies

The Adsorption script has the following dependencies:

- Python
- Atomic Simulation Environment (ASE) library

The ASE library is required for reading and writing structure files. It supports various file formats such as POSCAR, xyz, and cif. You can install the ASE library using pip:

```
pip install ase
```

1.5 Module Documentation

Here, we provide documentation for the Python module *Adsorption*. Author: Kazem Zhour

Date: 26.04.2024

Description: Adsorption of molecules on surfaces.
This Python script facilitates the adsorption of molecules onto surfaces, offering the flexibility to manipulate both the adsorption position and the orientation of the molecule.

Usage: This script requires input files for the surface and the molecule. The user will be prompted
to enter the filenames for these input files. Additionally, the script prompts the user to specify the origin and head atoms for defining the direction along the molecule, the angle for rotating the molecule around the z-axis, the atom of the slab on which to adsorb the molecule, and the desired adsorption height.

Dependencies: This script requires the Atomic Simulation Environment (ASE) library for reading and
writing structure files. ASE can handle various file formats such as POSCAR, xyz, and cif.

Example:
python3 Adsorption.py surface_file.vasp molecule_file.xyz –origine 0 –vertex 1 –adsorb_index 2 –height 3.5

This example demonstrates how to use the script to perform adsorption of a molecule on a surface. The user is prompted to input the filenames of the surface and molecule files, as well as the indices of the atoms defining the direction of the molecule. Then, the user specifies the index of the atom on the surface for adsorption and the desired adsorption height. The script generates an output containing the combined structure of the surface and the adsorbed molecule.

`Adsorption.`**`calculate_molecule_orientation`**`(`*molecule*, *origine*, *vertex*`)`

Calculates the orientation of the molecule based on user input.

Args:
molecule (ASE Atoms object): The molecule structure.

Returns:
phi (float): Azimuthal angle. theta (float): Polar angle.

`Adsorption.`**`main`**`()`

Main function to perform adsorption of molecules on surfaces.

`Adsorption.`**`read_input_files`**`(`*surface_file*, *molecule_file*`)`

Reads input files for surface and molecule.

Returns:
surface (ASE Atoms object): The surface structure. molecule (ASE Atoms object): The molecule structure.

Adsorption.**rotate_molecule**(*molecule*, *phi*, *theta*)

Rotates the molecule to align with the calculated orientation.

Args:

molecule (ASE Atoms object): The molecule structure. phi (float): Azimuthal angle. theta (float): Polar angle.

Adsorption.**translate_molecule**(*molecule*, *surface*, *adsorb_index*, *height*)

Translates the molecule to the adsorption site on the surface.

Args:

molecule (ASE Atoms object): The molecule structure. surface (ASE Atoms object): The surface structure. adsorb_index (int): Index of the adsorption site atom in the surface. height (float): Height of adsorption.

Below are some key functions provided by the *Adsorption* module:

Adsorption.**read_input_files**(*surface_file*, *molecule_file*)

Reads input files for surface and molecule.

Returns:

surface (ASE Atoms object): The surface structure. molecule (ASE Atoms object): The molecule structure.

Adsorption.**calculate_molecule_orientation**(*molecule*, *origine*, *vertex*)

Calculates the orientation of the molecule based on user input.

Args:

molecule (ASE Atoms object): The molecule structure.

Returns:

phi (float): Azimuthal angle. theta (float): Polar angle.

You can add more functions similarly.

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