

The movie.xyz output file

From GPUMD

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Brief Description

This file contains the positions (trajectory) of the atoms sampled at a given frequency.

The keyword which produces the current file

- `dump_position`

File format

- This is in the format of the XYZ (https://en.wikipedia.org/wiki/XYZ_file_format) file.
- Specifically, it reads:

```
number_of_atoms
frame_label
type_1 x1 y1 z1
...
number_of_atoms
frame_label
type_1 x1 y1 z1
...
```

Explanations

- The first line: `number_of_atoms` is the number of atoms for one frame.
- The second line: `frame_label` is the frame label (starting from 0) within a run.
- The third line: `type_1` is the atom type for atom 1 and `x1 y1 z1` are the position components (in units of angstrom) for this atom.
- Then there are `number_of_atoms - 1` remaining lines for the current frame.
- Then the pattern above is repeated.

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