
KMC Documentation

Release 1.0

David Abbasi

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INTRODUCTION

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KEYWORDS

2.1 How to read it

Keywords are written in bold. If the keyword needs a parameter, this parameter is written with `this font`. The kind of the parameter is defined after the point, where `.int` means that it is an integer, `.real` a real number, or `.str` a string. Sometimes, when the keyword is relative to a logical variable, the presence of the keyword switches its default value. If the parameter is [between brackets] it means that the parameter is optional. The (default value) is given in parenthesis. If the keyword is preceded with an exclamation sign means that this keyword is mandatory to be included in the input file.

2.2 Keywords

2.2.1 Mandatory keywords

- **! dimension** `dimension.int`

Set the size of the supercell (`dimension.int` x `dimension.int`). It must be bigger than 2

- **! deposition_rate** `deposition.real`

Set the deposition rate in ps^{-1}

- **! coverage** `coverage.real` (0-1)

Set the coverage of the surface. Values range from 0 to 1.

- **! number_of_kmc_steps** `steps.int`

Set the total number of steps of the simulation.

- **! barriers** `6 x barriers.real`

Set the energy barriers in eV. Descriptions of the barriers are shown in the table below.

#	Description
1	PTMDC diffusion via pivoting mechanism
2	PTMDC-PTMDC detachment (a dimer); then additive
3	PTMDC single isomerization
4	PTMDC extra barrier for assisted isomerization
5	PTMDC desorption from surface
6	PTMDC extra isomerization barrier for trans monomers

- **! temperature** `temperature.real`

Set the temperature of the simulation in Kelvin.

2.2.2 Detailing the simulations

- **ignore_single_HB**

If present, single hydrogen bond will not be taken into account.

- **seed** `seed.int`

Choose the seed for the random number generation. If `seed > 0` will use the given seed. If `seed <= 0` or not given, seed will be choose randomly.

- **do_testing**

If present, the program enters in the testing mode.

- **restart** `restartfile.str`

If present, KMC will restart from a previous calculation. The file `restartfile.str` must be given and must exist.

NOTE: In the testing mode can be generated an initial configuration of molecules, save that configuration to a file (option -2 in the testing mode) and choose that configuration as a restart file for run a entire simulation.

2.2.3 Printing and drawing keywords

- **printing** `printing.int` [0-5] (default = 0)

Set the level of print

- **show_site_numbers**

If present, numbers corresponding to the sites of the cell are drawn.

- **multicolor** (default = false)

If present, each isomer is filled with different colors.

Multicolor: (Inspired on the Day Of The Tentacle)

Cis : Blue rectangles, pink circles

L-trans: Magenta rectangles, green circles

D-trans: Green rectangles, yellow circles

- **drawing_frequency** `frequency.int` (default = 100)

Frames will be printed after `frequency.int` KMC steps.

- **drawing_scale** `scale.int` (default = 800)

Set the scale of the drawings in the frames.

- **drawing_title_size** `scale.int` (default = 20)

Set the size for drawing the title.

- **show_images** (default = false)

If present, files `.fig` are created.

- **no_jpgs** (default = false)

If present, the program will not generate the jpgs during the execution. After the simulation, jpgs images can be generated from `.fig` files executing

```
fig2dev -L jpeg frame.fig frame.jpg
```

If **show_images** is not present and **no_jpgs** is not present, then no frames will be created.

- **write_kmcout** [**formatted** (default = unformatted)] (default = false)

If present, kmc.out file will be written. By default it will be unformatted, but if the optional **formatted** keyword is present, it will be written in a human-readable form. This file contains the history of the entire simulation.

NOTE: kmc.out file becomes rapidly huge.

INDICES AND TABLES

- *genindex*
- *modindex*
- *search*