KMC Documentation

Release 1.0

David Abbasi

April 10, 2014

CONTENTS

Contents:

CHAPTER

ONE

INTRODUCTION

Lorem ipsum dolor sit amet, consectetur adipiscing elit. Etiam ac tortor lobortis, commodo est sit amet, vehicula nibh. Sed magna justo, adipiscing eget ante sit amet, tristique cursus enim. Donec dictum quam nunc, eu rhoncus nibh placerat mollis. Vestibulum vitae dignissim velit. Curabitur diam eros, dignissim ut eleifend in, tincidunt et lacus. Phasellus pharetra sapien a pellentesque tempus. Phasellus ullamcorper, risus a euismod dapibus, diam velit hendrerit eros, nec feugiat risus ipsum ut quam. Aenean varius eu diam sodales vulputate. Nunc vulputate felis ante, nec rutrum ligula volutpat pellentesque. Pellentesque habitant morbi tristique senectus et netus et malesuada fames ac turpis egestas. Curabitur pellentesque vestibulum scelerisque. Mauris lobortis euismod purus a adipiscing. Vestibulum aliquam ornare massa, in aliquam lectus fringilla at. Nullam et metus non est suscipit vulputate quis quis nisi.

Quisque quis venenatis metus. Nullam iaculis placerat neque, at pulvinar ligula ultricies eu. Fusce augue purus, mollis sit amet lacus in, interdum sagittis nisl. Vestibulum ante ipsum primis in faucibus orci luctus et ultrices posuere cubilia Curae; Pellentesque venenatis, ligula vitae porttitor fringilla, urna mi convallis odio, eget varius elit lacus eget sapien. Pellentesque habitant morbi tristique senectus et netus et malesuada fames ac turpis egestas. Cras sed faucibus dolor. Integer fringilla, odio vitae adipiscing ultricies, eros nulla cursus dui, vel commodo ante nibh at lectus. Maecenas vulputate dictum fringilla. In nibh sem, scelerisque vitae condimentum eu, hendrerit ac nibh. In hac habitasse platea dictumst.

Maecenas nec mi mauris. In hac habitasse platea dictumst. Nulla quis pulvinar ante. Praesent quis mi in lacus molestie fringilla non eget augue. Ut aliquam nulla eu auctor suscipit. Curabitur aliquet felis in enim auctor, malesuada ultricies orci varius. Pellentesque habitant morbi tristique senectus et netus et malesuada fames ac turpis egestas. Fusce molestie, urna pellentesque faucibus viverra, augue libero viverra eros, vel bibendum sem dui in lectus. Vivamus commodo purus vitae arcu lacinia, et accumsan nisi volutpat.

Etiam suscipit semper metus, a molestie metus aliquet condimentum. Maecenas congue varius rhoncus. Nam a orci aliquet, venenatis orci non, vestibulum diam. Suspendisse lobortis odio nec eros tincidunt consectetur. Maecenas sollicitudin facilisis ultrices. Maecenas fringilla ut tellus varius venenatis. Sed accumsan augue id felis varius facilisis. Pellentesque cursus a ligula id varius. Cras pharetra nisl enim, et eleifend eros pulvinar a. Nunc a luctus dolor. Curabitur laoreet justo rutrum, sagittis augue non, congue tortor. Pellentesque quis ipsum ac nulla vestibulum facilisis nec non libero. Suspendisse venenatis neque magna, a aliquam risus volutpat a. Ut in eleifend orci.

Sed pharetra leo eget libero aliquet aliquet. Nam sagittis nisl at tellus posuere, in commodo orci malesuada. Donec aliquet, metus sit amet mollis dictum, massa diam adipiscing lacus, sit amet egestas libero lacus quis ligula. Vivamus convallis sapien at quam adipiscing euismod eget at justo. In eu malesuada mi. Duis mattis sapien ut molestie consequat. Sed metus libero, eleifend nec enim sed, iaculis dapibus leo. Nunc hendrerit risus rhoncus rutrum scelerisque. Donec ornare aliquam enim dictum eleifend. Nulla facilisi. Maecenas eleifend volutpat urna at ultricies. Pellentesque facilisis scelerisque libero, molestie ultricies leo gravida nec. Nunc ut consectetur ante. Sed lacinia nunc nisl, at eleifend odio hendrerit quis. i

CHAPTER

TWO

KEYWORDS

2.1 How to read it

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

- ! **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 detachement (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.

- **do_testing**

If present, the program enters in the testing mode.

- **show_site_numbers**

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

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

  Set the level of print

- **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.

- **restart** `restartfile.str`

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

- **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.

CHAPTER

THREE

INDICES AND TABLES

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