

Zacros-post

Category

Software/Material Modelling

Authors

Dr Michail Stamatakis

Zacros-post is a post-processing and visualisation tool for kinetic Monte Carlo (KMC) software Zacros. It can visualise KMC simulation results and generate high-quality plots (to be used in publications) for the lattice structure, adsorbate configurations, reaction statistics and gas/surface species numbers.

Post-processing & visualization GUI for Zacros package for simulating molecular phenomena on catalytic surfaces

Product Specification

Zacros-post is a post-processing and visualisation tool for kinetic Monte Carlo (KMC) software [Zacros](#).

It can visualise KMC simulation results and generate high-quality plots (to be used in publications) for the lattice structure, adsorbate configurations, reaction statistics and gas/surface species numbers.

Description

Zacros-post is a graphical user interface (GUI) and library for post-processing and visualising output generated by the the graph-theoretical kinetic Monte Carlo software Zacros [<https://xip.uclb.com/product/zacros>]. The latter simulates the elementary processes of adsorption, desorption, diffusion and reaction on solids, for catalysis and surface science applications. Zacros-post can interactively post-process and visualise the contents of the output files generated by Zacros, thereby producing graphical representations of:

1. the lattice capturing the catalytic surface of the simulation,
2. the arrangement of adsorbates on the lattice as a function of time,
3. the statistics of occurrence of each elementary process,
4. the number of molecules adsorbed on the lattice for surface species as a function of time, and
5. the number of molecules consumed or produced for gas species.

The GUI can save plots of these results in png and pdf format to be used for publications. Moreover, the library files can be imported in Python projects, for further customisation in post-processing and plotting. The GUI is provided as a standalone application for Windows or Linux, and the library as compiled Python executables.

Usage Notes

When the user runs the program for the first time, it will prompt them to create a license request file for that machine. This file will have to be emailed to licensing@zacros.org (detailed instructions are given by the program at each step of the process). Then, the license file will be created and emailed back to the user (this can take up to 48 hours).

Licenses are not transferable between machines, and a user can only get as many licenses as they have paid for.

Tutorial

Post-processing and visualising results of KMC simulations can be tedious, time-consuming or prone to errors if done without a dedicated and validated software application. This tutorial explains how to install Zacros-post and provides a description of its main features:

<https://zacros.org/tutorials/17-zacros-post-processing>