

Zacros

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Kinetic Monte Carlo package for simulating molecular phenomena on catalytic surfaces

Product Specification

Zacros is an advanced kinetic Monte Carlo (KMC) software application written in Fortran 2003, for simulating the kinetics of molecular phenomena, such as adsorption and catalytic reactions, on surfaces.

Description

The software enables the first-principles prediction of catalytic performance metrics, such as activity and selectivity, as well as other experimental observables, such as the structure of adlayer phases or temperature desorption spectra. It employs the Graph-Theoretical KMC methodology, coupled with cluster expansion Hamiltonians and Brønsted-Evans-Polanyi relations for the adlayer energetics. This integrated implementation can naturally capture:

- steric exclusion effects for species that bind in more than one catalytic sites,
- complex reaction steps involving adsorbates in specific binding configurations and neighbouring patterns,
- spatial correlations and ordering arising from adsorbate lateral interactions that may involve many-body contributions,
- coverage effects, namely the dependence of the activation energy of an elementary event on the presence of spectators in the neighbourhood of this event.

In addition to these, the code features an easy-to-learn keyword-based language for defining a simulation, and can be run in “debugging” mode, thereby generating detailed output that can be used to efficiently troubleshoot a KMC simulation. The software comes with a manual, as well as exemplar input/output files. Informative articles, tutorials and examples that can help to get started with KMC can be found in the Zacros website: <http://zacros.org>.

Add-on: Zacros-post GUI

Zacros-post is a post-processing and visualisation tool for kinetic Monte Carlo (KMC) software Zacros and has a separate licensing page available at: <https://xip.uclb.com/product/zacros-post>

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.

Authors

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References

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<https://xip.uclb.com/product/Zacros>