Zacros 4.0

Zacros 4.0 is a Kinetic Monte Carlo (KMC) software package written in Fortran 2003, for performing non-equilibrium statistical mechanical calculations on lattice systems

Category
Software/Material Modelling

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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.

As of version 3.0, Zacros incorporates an MPI implementation of the Time-Warp algorithm for distributed (and exact) KMC simulations, making it possible to harness the computational power of massively parallel computing architectures.

As of version 4.0, Zacros implements advanced subgraph isomorphism algorithms (VF2, RI) that speed up calculations involving cluster expansions with complex or long-range patterns. Moreover, it features dynamic arrays that grow as-needed during the KMC simulation, new KMC state containers for the Time-Warp algorithm (optimized linked list and variable-element linked list compatible with dynamic arrays), and additional options for pseudo-random number generators (ACORN, xoshiro256**).

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.

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References

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