Zacros (30 day commercial evaluation)

Zacros 2.01 is a Kinetic Monte Carlo software package written in Fortran 2003, for simulating molecular phenomena on catalytic surfaces.-

Kinetic Monte Carlo package for simulating molecular phenomena on catalytic surfaces

Product Specification

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Description

The tool 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 for the adlayer energetics, which can naturally capture:

- steric exclusion effects for species that bind in more than one catalytic sites,
- complex reaction patterns involving adsorbates in specific binding configurations and neighbouring patterns,
- spatial correlations and ordering arising from adsorbate lateral interactions that involve many-body contributions.

Zacros features an easy-to-learn keyword-based language for defining a KMC simulation, and can be run in “debugging” mode, thereby generating detailed output that can be used for efficient troubleshooting. The package comes with a manual, as well as exemplar input/output files.

Training

Optional training can be arranged with the program author through our partner organisation UCL Consultants Ltd. For information on rates and availability, please contact them on 020 7679 9794 or info@uclconsultants.com quoting "XIP product Zacros".

Commercial Evaluation

The version of Zacros made available under the Commercial Evaluation Licence is Windows executable functional for 30 days. If after the trial period a perpetual licence is required please visit https://xip.uclb.com/product/Zacros.

References

1. Vlachos, Stamatakis(2011) , http://scitation.aip.org/content/aip/journal/jcp/134/21/10.1063/1.3596751, Journal of Chemical Physics, 134(21), 214115
2. Stamatakis, Hetherington, d’Avezac, Nielsen(2013) , http://dx.doi.org/10.1063/1.4840395, Journal of Chemical Physics, 139(22), 224706

Category

Software/Material Modelling

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