Title:

From Energetics to Rates: A Hands-on Workshop on Microkinetic Modelling with ML Potentials

Presenters

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Abstract

Linking atom-scale energetics to macroscopic reaction rates remains a central challenge in heterogeneous catalysis. This half-day, hands-on workshop bridges that gap by taking participants from adsorption and reaction energetics to working microkinetic models. In the morning, attendees use Python/ASE to build surface slabs, define adsorption sites, and run accelerated geometry optimisations with state-of-the-art machine-learned interatomic potentials, integrating these with conventional electronic-structure workflows where appropriate. In the afternoon, they assemble simplified 6–10-step reaction networks, derive transition-state-theory rate expressions, and solve mass-balance ODEs to obtain coverages, turnover frequencies, and sensitivity metrics such as degree-of-rate-control. Throughout, we emphasise practical high-performance computing on CHPC. Participants leave with a functional microkinetic model for a reaction network of their choice, diagnostic visualisations, and a clear roadmap for extending to more complex chemistries. Designed for graduate students, postdocs, and early-career researchers with basic Linux command-line experience and introductory Python skills, the workshop prioritises conceptual clarity without overwhelming computational detail. In the South African context, where catalysis underpins Fischer–Tropsch fuels, ammonia synthesis, and emerging green-chemistry value chains, building local expertise in microkinetic modelling will help accelerate innovation in sustainable processes. By leveraging CHPC's computational backbone and training a critical mass of practitioners, this workshop cultivates national capacity in computational catalysis and equips researchers to translate elementary-step energetics into predictive, rate-based insights that inform catalyst design and deployment.

Target audience & prerequisites: Graduate students, postdocs, and practitioners in catalysis/materials/chem-eng; basic Linux command line and introductory Python.

Format: Tutorial + guided lab + "troubleshooting clinic".

Duration: **Half day**, **Sunday 30 Nov 2025** (CHPC workshop day).

Detailed Plan and Suggestions

Workshop Schedule

Time	Activity
09:00 – 09:30	Reaction networks and energetics (lecture/theory)
09:30 – 10:00	Microkinetic modeling principles (lecture/theory)
10:00 – 11:00	Defining a reaction system & computing energetics (hands-on)
11:00 – 12:00	Constructing & running microkinetic models (hands-on)
12:00 – 12:30	Reflection, interpretation, and Q&A

Lecture 1 (30 min): Reaction Networks and Energetics

- Fundamentals of adsorption, reaction, and desorption thermodynamics
- Building slab models: periodic cells, adsorption sites, and coverage effects
- Overview of machine-learned potentials (e.g., GAP, MTP, NequIP) for rapid energy evaluation
- Hands-on demo: ASE scripts to relax adsorbates with a pretrained potential

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Lecture 2 (30 min): Microkinetic Modeling Principles

- Writing elementary step lists and rate expressions based on transition state theory
- Setting up mass-balance ODEs for coverage and rate calculations
- Importance of kinetic pathways, degree of rate control, and sensitivity analysis
- Introduction to Python frameworks (CatMAP, Cantera, custom scripts) for solving kinetic networks

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Special requirements:

- Attendees bring laptops (Linux/macOS/WSL).

- Reliable Wi-Fi, Internet access and projector.
- CHPC cluster access during the session (temporary/guest accounts or instructions for using personal CHPC accounts).

Tools and Best Practices

- We will provide a Conda / Docker environment with pre-installed ASE, CatMAP, scikit-learn, and Jupyter notebooks
- Use CHPC's scheduler: sample job scripts for DFT/ML potential calculations and kinetic runs
- Prepare template input files for common surfaces (Pt(111), Cu(111), etc.) and reaction steps
- Encourage small teams to share tasks: one computes energetics while the other codes the microkinetic model
- Supply a GitHub repository with step-by-step guides, annotated notebooks, and example data
- Recommend interactive plotting (Plotly) for real-time analysis of coverage and turnover frequency

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Learning outcomes

Participants will be able to:

1. compute and curate adsorption/barrier data with ASE+MLIPs;
2. assemble and solve compact microkinetic models;
3. interpret TOF/coverage and degree-of-rate-control results;
4. run and manage small high-throughput energetics campaigns on CHPC

Suggested Reaction Systems and Catalyst Surfaces

Reaction System	**Catalyst Surface**
CO oxidation: $CO + ½ O_2 \rightarrow CO_2$	Pt(111)
Water-gas shift: $CO + H_2O \rightarrow CO_2 + H_2$	Cu(111)
CO_2 hydrogenation to methane: $CO_2 + 4 H_2 \rightarrow CH_4 + 2 H_2O$	Ni(111)
Methanol synthesis: $CO_2 + 3 H_2 \rightarrow CH_3OH + H_2O$	Pd(111)
Ammonia synthesis: $N_2 + 3 H_2 \rightarrow 2 NH_3$	Ir(111)
Ethylene hydrogenation: $C_2H_4 + H_2 \rightarrow C_2H_6$	Rh(111)
Benzene hydrogenation: $C_6H_6 + 3 H_2 \rightarrow C_6H_{12}$	Pd(111)
NO reduction: $2 NO + 2 CO \rightarrow N_2 + 2 CO_2$	Rh(111)
Formic acid decomposition: $HCOOH \rightarrow CO_2 + H_2$	Ag(111)
Methane activation: $CH_4 \rightarrow CH_3 + H$	Au(111)