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

Sunday, 30 November 2025 09:00 (1h 30m)

Linking atomistic energetics to macroscopic rates remains a core challenge in heterogeneous catalysis. This full-day, hands-on workshop takes participants from surface slab setup and adsorption energies (Python/ASE) to working microkinetic models. We use machine-learned interatomic potentials to approximate energetics, then build reaction networks, derive transition-state-theory rate expressions, and solve mass-balance ODEs to obtain coverages, turnover frequencies, and degree-of-rate-control sensitivities. Practical HPC on CHPC is woven throughout. Attendees leave with a functional model for a reaction of their choice and a clear roadmap to extend it.

Presenting Author

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Student or Postdoc?

No. Not a student nor Postdoc.

Institute

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Registered for the conference?

Yes

CHPC User

Yes

CHPC Research Programme

MATS1516 and CHEM0780

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