Automated and high-throughput reactivity analysis in homogeneous catalysis
The deactivation complexity of Mn(I) hydrogenation catalysts

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DOI
10.4233/uuid:610c0657-9706-4fde-90ce-6bc9ecd14620

Publication date
2023

Document Version
Final published version

Citation (APA)
Hashemi, A. (2023). *Automated and high-throughput reactivity analysis in homogeneous catalysis: The deactivation complexity of Mn(I) hydrogenation catalysts*. [Dissertation (TU Delft), Delft University of Technology]. https://doi.org/10.4233/uuid:610c0657-9706-4fde-90ce-6bc9ecd14620

Propositions

accompanying the dissertation

AUTOMATED AND HIGH-THROUGHPUT REACTIVITY ANALYSIS IN HOMOGENEOUS CATALYSIS: THE DEACTIVATION COMPLEXITY OF MN(I) HYDROGENATION CATALYSTS

by

Ali HASHEMI

1. Knowledge is not necessarily power.
2. While most of the efforts in catalysis research are implicitly dedicated to the “known” conditions/mechanisms, exploring the “unknowns” is key to breakthroughs. (We have only touched the tip of the iceberg in view of this)
3. Clear measures are necessary to distinguish when our autogenerated CRNs are satisfactorily complete and accurate to answer physical questions raised. In other words, we should know "When should we stop?" (*I. Ismail, R. Chantreau Majerus, S. Habershon, J. Phys. Chem. A 2022, 126 7051–7069*)
4. AI/ML approaches to in silico catalyst research and development naturally inherit the underlying inaccuracies of the ab initio method used for their training. (Chapter 4)
5. Automated high throughput calculations should be monitored since exhaustive reaction sampling may become more wasteful than actual experiments. (Chapter 4)
6. Modern peer review process is critical for ensuring high quality publications.
7. It helps the PhD trajectory a lot, if supervisors are experts on the projects they choose to lead.
8. While scientifically beneficial, extra care should be given when deciding on putting engineers and scientists to work together.
9. Part time remote working should be considered as a serious alternative in view of environmental impacts given that proper personal and professional socializing measures are not neglected.
10. Openness towards interdisciplinary collaborations (and the acceptance culture required for such work) are vital to creative academic research.

These propositions are regarded as opposable and defendable, and have been approved as such by the promotors prof. dr. E. Pidko and prof. dr. M.P. Gaigeot.