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Propositions

accompanying the dissertation

THE WONDERS OF DIGITAL CATALYSIS BRIDGING CHEMISTRY AND MACHINE LEARNING FOR HOMOGENEOUS CATALYST DESIGN

by

Adarsh Kalikadien

1. Artificial intelligence will not transform chemistry through larger datasets or models alone; its value lies in automated, modular pipelines linking data generation and analysis (Chapter 1 and 8).
2. In small datasets, apparent correlations between computational descriptors and catalyst performance may be spurious, and rigorous validation is essential before claiming predictive utility for such statistical models (Chapter 2).
3. Accurate predictive modeling in homogeneous catalysis requires balancing computational cost with descriptor accuracy, while explicitly accounting for the dynamic flexibility of catalysts (Chapters 3-6).
4. When used without understanding the underlying training data or algorithms, machine learning interatomic potentials generate misleading artefacts rather than reproducible discoveries (Chapter 7).
5. The hiring and selection of academic staff, particularly future professors, should emphasize didactic ability, empathy, and the substantive content of their scientific work over research metrics.
6. Science, Technology, Engineering and Mathematics (STEM) curricula that do not provide a solid foundation in statistics, programming, and data science fail to prepare students for the realities of modern scientific research.
7. Open Science practices remain undervalued due to the lack of tangible incentives in the current academic system.
8. Mastery of political skills, such as negotiation, networking and public speaking, must be an integral part of scientific training.
9. First-generation students and scientists face structural disadvantages in academia, as their environments often lack the cultural capital to navigate academic systems.
10. Those who cling rigidly to religious rules often reveal a limited understanding of the deeper teachings of their own faith.

These propositions are regarded as opposable and defensible, and have been approved as such by the promoters prof. dr. E. A. Pidko and prof. dr. B. Dam.

Stellingen

behorend bij het proefschrift

THE WONDERS OF DIGITAL CATALYSIS BRIDGING CHEMISTRY AND MACHINE LEARNING FOR HOMOGENEOUS CATALYST DESIGN

by

Adarsh Kalikadien

1. Kunstmatige intelligentie zal de chemie niet transformeren door alleen grotere datasets of modellen; de werkelijke waarde ligt in geautomatiseerde, modulaire pipelines die datageneratie en analyse verbinden (Hoofdstukken 1 en 8).
2. In kleine datasets kunnen correlaties tussen computationele descriptoren en experimentele katalysatorprestaties misleidend zijn; strikte validatie is onmisbaar (Hoofdstuk 2).
3. Nauwkeurige modellering in homogene katalyse vereist een balans tussen rekenkosten en computationele descriptor-nauwkeurigheid, met expliciete aandacht voor conformationele flexibiliteit (Hoofdstukken 3-6).
4. Zonder begrip van trainingsdata of algoritmen leveren machine learning interatomaire potentialen misleidende artefacten op in plaats van reproduceerbare inzichten (Hoofdstuk 7).
5. Selectie van academisch personeel, vooral hoogleraren, moet meer gebaseerd zijn op didactiek, empathie en inhoudelijke kwaliteit dan op kwantitatieve indicatoren.
6. Curricula van bèta opleidingen zonder basis in statistiek, programmeren en datawetenschap bereiden studenten onvoldoende voor op modern onderzoek.
7. Open Science blijft ondergewaardeerd zolang structurele prikkels in het academisch systeem ontbreken.
8. Politieke vaardigheden zoals onderhandelen, netwerken en spreken in het openbaar moeten integraal deel uitmaken van wetenschappelijke vorming.
9. Eerste-generatiestudenten en -onderzoekers ervaren structurele achterstanden doordat hun omgeving vaak het culturele kapitaal mist om academische systemen te navigeren.
10. Wie zich rigide vastklampt aan religieuze regels onthult vaak een beperkt inzicht in de diepere beginselen van de eigen geloofstraditie.

Deze stellingen worden oponeerbaar en verdedigbaar geacht en zijn als zodanig goedgekeurd door de promotoren prof. dr. E. A. Pidko and prof. dr. B. Dam.