



Universiteit
Leiden
The Netherlands

Accurate modeling of the dynamics of dissociative chemisorption on metal surfaces

Gerrits, N.

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Propositions

accompanying the thesis

“Accurate Modeling of the Dynamics of Dissociative Chemisorption on Metal Surfaces”

- i. The minimum barrier does not determine the probability of a molecule-metal surface reaction, rather the entire dynamically relevant potential energy surface does. (Chapters 3-10)
- ii. Neural network potentials allow for accurate computational theoretical studies, which would otherwise have been intractable. (Chapters 3 and 8)
- iii. GGA density functionals are not suitable for molecule-metal surface reactions when a large amount of charge transfer occurs at the TS, which is generally the case when the difference between the surface's work function and the molecule's electron affinity is smaller than 7 eV. (Chapter 5)
- iv. Single atom alloys have the potential to alter chemistry on a local level and advance heterogeneous catalysis in a complex fashion. (Chapter 7)
- v. Computed sticking probabilities are often not what they seem, since many theoreticians neglect the contribution of rovibrational excitation in a molecular beam. (G.J. Kroes, *Phys. Chem. Chem. Phys.*, vol. 23, no. 15, pp. 8962–9048, 2021)
- vi. More experiments are required that verify existing molecule-metal surface reaction experiments since too often $n = 1$ is treated as good science. (L. Österlund et al., *Phys. Rev. B*, vol. 55, no. 23, pp. 15452–15455, 1997; M. Kurahashi and Y. Yamauchi, *Phys. Rev. Lett.*, vol. 110, no. 24, p. 246102, 2013)
- vii. Jacob's ladder is outdated, inconsistent, and unable to distinguish several important features of density functionals, and, therefore, should not be used anymore. (J. P. Perdew and K. Schmidt, *AIP Conf. Proc.*, vol. 577, no. 1, pp. 1–20, 2001)
- viii. AIMD and (Q)CT are commonly mistaken as two separate approaches that do not overlap. AIMD and (Q)CT are similar to the cow and animal analogy: In practice, with AIMD one (almost) always runs (Q)CT, but with (Q)CT one does not always use AIMD. (M. Karplus et al., *J. Chem. Phys.*, vol. 43, no. 9, pp. 3259–3287, 1965)
- ix. It is unreasonable to put most, or any at all, of the PhD defense costs on a PhD student since the university receives about 80,000 euros for a successful PhD defense. (A. de Vries-Stotijn, “Science under pressure: The PhD premium – Quantity over quality,” Tilburg University, pp. 35-43, 2019)
- x. As the analysis of reaction mechanisms is becoming increasingly more complex, the required number of figures visualizing the reaction mechanism will increase. Hence, the printing cost of a thesis detailing reaction mechanisms is to be expected to increase rapidly as well.
- xi. Alleen een radicaal totaalplan kan de woningmarkt nog laten terug keren naar een wenselijke situatie. Zo'n plan zou onder andere afschaffing van de verhuurdersheffing en hypotheekrenteaftrek, uitbreiding van het puntensysteem naar de vrije sector, verwijdering van het aandeel van de WOZ-waarde in het puntensysteem, omkeer van de decentralisatie van de overheid, substantiële verkleining van de agrarische sector, en verwijdering van de optie op tijdelijke huurcontracten bevatten.
- xii. Replying “yes” or “no” to a multiple-choice question can be acceptable. (G. W. Scragg, “Problem Solving with Computers”, Jones & Bartlett Publishers, London, p. 310, 1996)