Surface temperature and the dynamics of H2 on Cu(111)

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Stellingen

Behorende bij het proefschrift

Surface Temperature and the Dynamics of H_2 on Cu(111)

i. The effects of surface temperature on the dissociation of H_2 on and its scattering from Cu(111) need to be considered in computational models to reproduce experimental results accurately. (Chapter 3, 5, and 6)

ii. The effect of a (thermally) distorted surface on the H_2/Cu(111) surface interaction can be described using just five distorted surface atoms. (Chapter 4)

iii. For an H_2 molecule reacting with Cu(111), constraining the molecule to a 1×1 unit cell during dynamics is sufficient to describe both dissociation and scattering accurately with the SCM. (Chapter 4-6)

iv. Not only the energetic height but also the geometrical shape of the reaction barrier is vital for an accurate description of molecule-metal dissociation reactions. (Chapter 3-6)

v. To accurately describe a molecule-metal system in its entirety, descriptions at a quantum dynamical level must be used. (Bin Jiang and Hua Guo, *J. Chem. Phys* **150,** 180901 (2019))

vi. Due to the ever increasing accuracy of computational models, contributions that were once considered negligible will eventually become important. (Geert-Jan Kroes and Cristina Díaz, *Chem. Soc. Rev.* **45**, 3658 (2016))

vii. The quality of published results, and the accurate and careful documentation of scientific code and its input data are equally important. (Roger D. Peng, *Science* **334**, 1226-1227 (2011))

viii. Although the GOTO statement can in many ways lead to less structured code, its use should not be completely disregarded as unclear. (Donald E. Knuth, *ACM Computing Surveys* **6.4** (1974))

ix. De werkdruk die gepaard gaat met het geven van onderwijs binnen het LIC kan sterk verminderd worden door een meer actieve toepassing van student-assistenten.

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