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Hydrogen dissociation on metal surfaces

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PROPOSITIONS

accompanying the thesis

“HYDROGEN DISSOCIATION ON METAL SURFACES”

- i. The broadening of reaction probability curves with surface temperature can be explained by the static corrugation arising from instantaneous displacements in the surface. (Chapter 3)
- ii. The experimental reaction and diffraction probabilities for H₂ dissociation on Ru(0001) seem to be inconsistent with each other. (Chapter 4)
- iii. Functionals with a van der Waals correction can give an improved description of molecule–surface reactions. (Chapters 4 and 6)
- iv. It is striking how, despite a large energy transfer in a collision of hydrogen with a CO-covered surface, there is only a small effect on reaction. (Chapter 7)
- v. To obtain a proper description of both the surface and the molecule–surface interaction for a molecule–surface system with DFT it is likely that at least a meta-GGA functional is required.
(J. P. PERDEW *et al.* *Phys. Rev. Lett.* **103**(2), 026403, 2009)
- vi. The large variety of existing exchange–correlation functionals makes it almost necessary to have a library of functionals available.
(M. A. L. MARQUES *et al.* *Comp. Phys. Comm.* **183**(10), pp. 2272–2281, 2012)
- vii. For a good description of surface temperature in dynamics calculations, more than one degree of freedom of the surface is needed.
(M. BONFANTI *et al.* *Z. Phys. Chem.* **227**(11), pp. 1397–1420, 2013)
- viii. The biggest source of errors in calculations on hydrogen dissociation on metal surfaces is probably the chosen exchange–correlation functional.
- ix. It is important in scientific literature to indicate for DFT calculations unambiguously which exchange–correlation functional is used.
- x. Many programming errors in programs written in FORTRAN start with logical assumptions about how the language works.
- xi. Privatisation of public transport is not only a *contradictio in terminis*, it is also mostly not in the interest of the traveler.