Hydrogen dissociation on metal surfaces: A semi-empirical approach

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Propositions

1. Barrier heights for H_2-metal surface reactions are highly dependent on the choice of exchange-correlation functional. (Chapter 3)
2. In the context of the vdW-DF functionals, the term local and non-local are often used in the literature, and in the DFT community, the dispersion energy is understood as an inherently non-local property. (S. Grimme, Comput. Mol. Sci. 1, 211 228 (2011))
3. Including non-local vdW-DF2 correlation in the exchange-correlation functional improves the description of weakly activated dissociation of H_2 on Pt(111) and gives a proper width of the reaction probability as a function of incidence energy. (Chapter 3)
4. The enhancement of the reactivity upon molecular vibrational excitation for late barrier systems is due to the conversion of part of the vibrational energy into translational energy in the direction of the reaction coordinate. (D. Halstead and S. Holloway, J. Chem. Phys. 93, 2859 (1990))
5. GGA functionals are not good at giving a simultaneously accurate description of molecule-surface interaction energies and metal surfaces. Meta-GGA functionals are more accurate and can give both a good description of molecule-surface interaction as well as the surface itself. (L. Schimka et al Nature Mater. 9, 741-744 (2010))
6. The inverse relationship between reaction and collision energy at low energy in H_2 + Pt(211) is due to trapping in a weak molecular chemisorption well. (D. A. McCormack et al, J. Chem. Phys. 122, 194708 (2005))
7. When using the DF2-functional in the description of the dynamics of molecular hydrogen on Pt(211), the trapping mechanism may become more substantial, which may affect the computation of sticking probabilities for slow molecules. (Chapter 5)
8. There is no direct way to measure barrier heights, the best way of determining them is by a close comparison of molecular beam experiments and dynamics calculations reproducing the reaction probability measured therein. (Chapter 6)
9. Chemically accurate theoretical descriptions can be obtained on the basis of the specific reaction parameter approach to density functional theory, allowing reaction barriers to be obtained with chemical accuracy. However, being semi-empirical this approach suffers from two basic problems. (Chapter 6)
10. Scientific beliefs must be evaluated and supported by empirical data.
11. Theories cannot be "verified", but they can be "confirmed", "warranted", or "falsified".