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Semi-empirical approach to the simulation of molecule-surface reaction dynamcis

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Propositions

i. It is not easy to predict and to intuitively explain the behavior of a density functional.
– Chapter 3

ii. Barrier heights cannot be measured directly, and are best determined through a close comparison of molecular beam experiments and dynamics calculations reproducing the reaction probability measured therein.
– Chapter 4

iii. The reasons why the two functionals (PBE and SRP32-vdW) predict such different reactivity for CHD_3 on Pt(111) are related to the presence of van der Waals correlation in the SRP32-vdW functional, which is absent from the PBE functional.
– Chapter 6

iv. The HOD molecule can react regardless of its initial orientation and large changes in the values of the angle θ are observed on the molecule's way to the surface.
– Chapter 7

v. In principle the SRP-DFT-AIMD approach should be applicable to any molecule reacting with a metal surface, as long as experiments can be devised on the system that are amenable to an accurate quasiclassical dynamical treatment.
– Nattino *et al.*, *J. Phys. Chem. Lett.*, 7, 2402 (2016)

vi. The CHD_3 molecule does not react by relaxing the reactive bond along the angle θ, but rather by changing the orientation of the umbrella axis after passing through a reactive gate.
– Füchsel *et al.*, *Phys. Chem. Chem. Phys.*, 18, 8174, (2016)

vii. The AIMD method allows the calculation of statistically accurate dissociation probabilities without the need of introducing *a priori* dynamical approximations concerning the evolution of specific molecular degrees of freedom or concerning the role played by surface atom motion.
– Nattino *et al.*, *J. Chem. Phys.*, 144, 044702 (2016)

viii. The dissociation of small polyatomic molecules on transition metal surfaces often represents the rate limiting step in the heterogeneously catalyzed processes used to produce chemicals on an industrial scale. Developing a predictive understanding of these dissociation reactions is not only of fundamental interest but also of practical importance.
– Chadwick *et al.*, *J. Chem. Phys.*, 148, 014701 (2018)

ix. Answers are always limited, temporary, unsatisfactory. Questions, on the other hand, are the true engine of mental activity: a person who does not ask questions, or who is satisfied with the answers, cannot go very far.
"Le risposte sono sempre limitate, provvisorie, insoddisfacenti. Le domande invece sono il vero motore dell'attività mentale: un uomo che non si pone domande, o che si contenta delle risposte, non va molto lontano."
– Piero Angela, Da zero a tre anni, *Mondadori*, (2017)