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Beyond the Born-Oppenheimer static surface model for molecule-surface reactions

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Citation

Spiering, P. (2019, December 16). *Beyond the Born-Oppenheimer static surface model for molecule-surface reactions*. Retrieved from <https://hdl.handle.net/1887/81817>

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Title: Beyond the Born-Oppenheimer static surface model for molecule-surface reactions

Issue Date: 2019-12-16

Propositions

accompanying the thesis

“Going Beyond the Born-Oppenheimer Static Surface Model for Molecule-Surface Reactions”

- i. **The effect of surface motion on the reaction probability of H₂ on Cu(111) can be taken into account with chemical accuracy using simple analytic functions with only a few fitting parameters.** (Chapter 3)
- ii. **Molecular dynamics with electronic friction based state-to-state scattering of H₂ from Cu(111) suggests a fingerprint of non-adiabatic effects that can be used for experimental verification of non-adiabatic models.** (Chapter 4)
- iii. **Electron-hole-pair excitation can significantly affect the reaction probability for some systems and can thus not be neglected *a priori*.** (Chapter 5)
- iv. **Considering the transformation rules of tensors under coordinate transformations and comparing them with the consequences of symmetry constraints allows for a clear path towards extending symmetry adapted machine learning methods for scalar values to tensors.** (Chapter 6)
- v. **State-of-the-art machine learning algorithms are not yet able to accurately learn physics and chemistry without the guidance of a human being.** (arXiv:1807.10300 [quant-ph])
- vi. **It is necessary to take non-adiabatic effects into account when designing new (semi-)empirical functionals.**
- vii. **There are still many details to be scrutinized before electronic friction can be used as-is.**
- viii. **While quantum supremacy may supersede all previous effort to find suitable approximations for modeling molecule-surface reactions, the fundamental insights gained from classically constrained computations still remain useful.** (Phys. Chem. Chem. Phys., 2019,21, 15356-15361)
- ix. **One can encounter a lot of friction when working with scientists.** (Finney B. (1991) Scientists and Seamen. In: Harrison A.A., Clearwater Y.A., McKay C.P. (eds) From Antarctica to Outer Space. Springer, New York, NY)
- x. **When you automate your workflow, you ensure that when you make a mistake, you make it consistently and reproducibly.** (2016 IEEE International Conference on Big Data (Big Data), Washington, DC, 2016, pp. 3045-3051.)
- xi. **Having a window with a view to a garden can improve productivity, however, this is countered by bunnies hopping around in said garden.** (Environ. Sci. Technol. 2010, 44, 10, 3947-3955 and Applied Ergonomics, 4 (1) (1973), pp. 19-22)