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Photoinduced processes in dye-sensitized photoanodes under the spotlight: a multiscale in silico investigation

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Propositions

For the Thesis

‘Photoinduced Processes in Dye-Sensitized Photoanodes under the Spotlight – A Multiscale in Silico Investigation’

- i) The resonances between electronic coherences and nuclear vibrations required for photoinduced coherent charge transfer can be shifted by isotope exchange. (Chapter 3)
- ii) Photoinduced coherent charge transfer requires symmetry breaking and involves concerted angular motion in the electronic and nuclear subsystems. (Chapter 2 and 3)
- iii) Nuclear dynamics and trajectory averaging are crucial to adequately describe photoinduced electron injection processes in dye-sensitized photoanodes. (Chapter 4)
- iv) Combining geometries and frequencies obtained by a tight binding approach with the electronic energy by DFT allows for quick, reliable determination of the catalytic cycle and Gibbs free energies for a water oxidation catalyst in agreement with experiment. (Chapter 5)
- v) *In Silico* design and optimization of molecular components can provide explicit guidelines for D- π -A structured charge separators, such as optimal spacer length and breaking of conjugation.
- vi) Modern semi-empirical methods in combination with quantum-classical simulations now allow for investigations of photoinduced processes in large, extended and embedded systems.
- vii) A photon is a selective reaction partner that we should take more advantage of: it can provide energy in a directional, non-statistical, thus non-Arrhenius way, driving chemical reactions.
- viii) Artificial and natural photosynthesis, as well as life and societal progress are a never-ending fight against equilibrium.
- ix) While artificial photosynthesis shows great potential in mitigating climate change, the real challenge is political in nature and requires the crack-down on corruption, euphemistically called lobbying.
- x) If your official agenda is progress and freedom, pseudo-monarchic and aristocratic structures and symbols are a curious way of expressing this.