Coupled electronic and nuclear dynamics at interfaces of artificial photosynthesis devices

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Stellingen
Behorende bij het proefschrift:
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1. When immobilized on a surface or incorporated into an artificial enzyme, the performance of the Ru-bda water oxidation catalyst is limited (Chapter 4).

2. The performance of cobalt porphyrins as hydrogen evolution catalysts is enhanced by functionalizing the ligand with electron-withdrawing substituents (Chapter 5).

3. Immobilization of the P1 dye on NiO leads to at least two distinct surface species (Chapter 6).

4. The weak vibronic coupling observed for specific terrylene molecules on hexagonal boron nitride can be attributed to physisorption of the molecule on charge-donating defect sites (Chapter 7).

5. Non-adiabatic effects considerably affect the dynamics of proton-coupled electron transfer in both natural and artificial photosynthetic systems.

6. Nuclear motion plays a critical role in the photoinduced charge separation dynamics at dye-semiconductor and catalyst-dye interfaces.

7. The over-delocalization of electron and hole densities by the commonly used GGA-DFT functionals substantially impacts the dynamics observed in DFT-based molecular simulations.

8. Machine learning strategies offer a promising approach to extending the timescales of molecular dynamics simulations while maintaining ab initio-quality interatomic potentials.

9. Artificial photosynthesis might ease policy making in the future, but it does not alleviate the responsibility on politicians to act now.

10. It is critical for successful climate policy that action is taken in a fair manner.

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