Water on rutile (110): A 5 dimensional wave packet dynamics study of photocatalysis

Jan-Erik Oest[a] and Thorsten Klüner[a]

[a] *Institute of Chemistry, Carl von Ossietzky University Oldenburg, 26111 Oldenburg, Germany*
jan-erik.oest@uol.de

Accurate and efficient high-dimensional wave packet dynamics are crucial for understanding quantum mechanical phenomena and receiving state resolved expectation values. Especially for photocatalytic reactions exact quantum dynamics are used to get insight into reaction pathways. High dimensional studies of large systems such as molecules on semiconductor surfaces require a lot of care to select the right parameters, which describe the system in its entirety but at the same time keep the demand on computational resources as low as possible. With high dimensional potential energy surfaces already existing for the system of H_2O on TiO_2 rutile (110) [1], we aim to study the dynamics of photodesorption and -dissociation of the water molecule in detail to gather knowledge about the mechanisms surrounding photocatalytic water splitting on titanium dioxide.

References

1. J. Mitschker and T. Klüner, *J. Theor. Comput. Chem.* **15** (2016), 1650013.