Ab initio modelling of defective titania surfaces

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Defects and their electronic structures in titania play important roles to many intriguing phenomena such as photocatalysis and defect magnetism. Using density functional theory methods, we investigate the interplay between defect-induced polaron and water on titania surfaces. On one hand, we find the adsorption of molecules such as water and methanol leads to a segregation of polaron across the surface [1]. Our calculations are in line with scanning tunnelling microscopy and photo-spectroscopy measurements [1]. On the other hand, we reveal the explicit role of polaron on water dissociation. We further investigate the electronic structure of original oxygen vacancy defects using *ab initio* correlated wave function approaches, and find position dependence of spin states in oxygen vacancies.

References:
[1] Chi M. Yim, Ji Chen, Yu Zhang, Bobbie-Jean Shaw, Chi L. Pang, David C. Grinter, Hendrik Bluhm, Miquel Salmeron, Christopher A. Muryn, Angelos Michaelides, and Geoff Thornton. Submitted.