Defects and dynamics at oxide surfaces from first principles

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First principles simulations have had a major impact on our understanding of the physical and electronic structure of oxide surfaces. The low index surfaces of TiO_2 have emerged as the paradigm system for these studies. This is in part due to the enormous technological importance of titania powders but also because of the flexibility of its stochiometry, electronic and physical structure which make it ideal for systematic studies. We will report the results of extensive first principles calculations on the surface chemistry, defect structures and dynamical effects at the (110) and (100) surfaces.