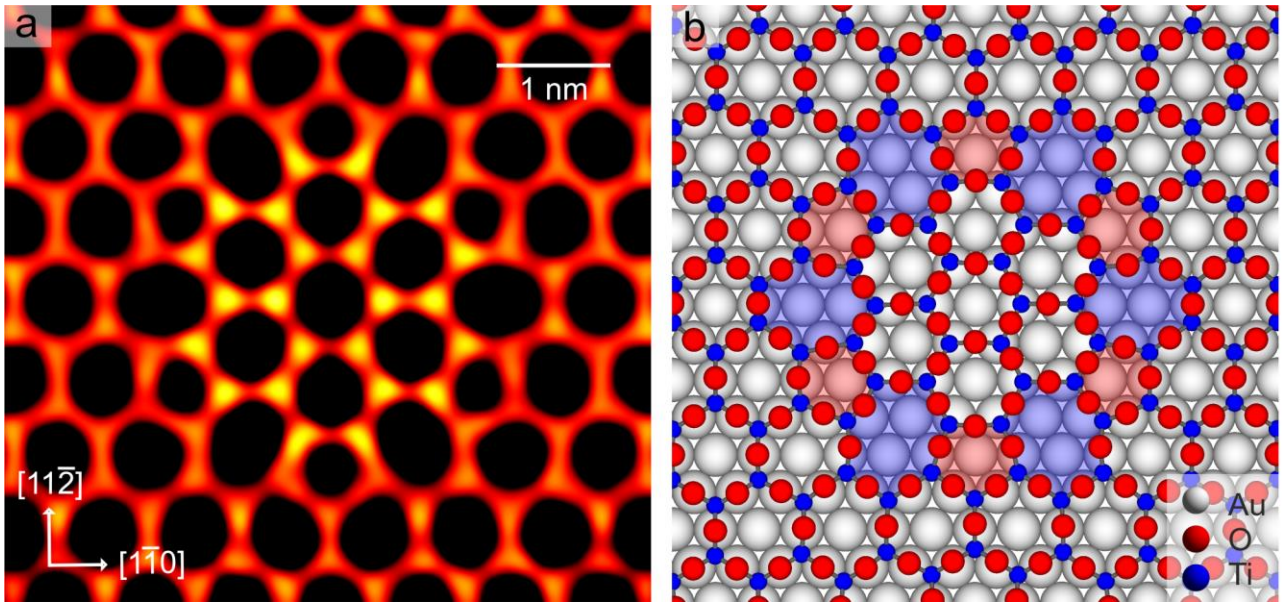
Defects in Monolayer Films of Ti_2O_3 on Au (111)

Shuqiu Wang[1], Xiao Hu[1], Jacek Goniakowski[2, 3], Claudine Noguera[2, 3], Martin R. Castell[1]

[1]*Department of Materials, University of Oxford, Parks Road, Oxford, OX1 3PH, U.K.*
[2]*CNRS, Institut des Nanosciences de Paris, UMR 7588, 4 place Jussieu, 75005 Paris, France*
[3]*UPMC Univ Paris 06, INSP, UMR 7588, 4 place Jussieu, 75252 Paris CEDEX, France*
shuqiu.wang@materials.ox.ac.uk

Defects in monolayer oxides can modify the properties of the films, leading for example to novel properties such as enhanced chemical reactivity. By a combination of scanning tunneling microscopy (STM) and density functional theory (DFT), we investigate defects in monolayer films of Ti_2O_3 supported on Au(111). The Ti_2O_3 films have a (2×2) honeycomb structure that demonstrates a high structural flexibility and is an ideal template for metal atom adsorption [1]. A rich variety of intrinsic defects including Ti and O vacancies, a Stone-Wales defect, closed-loop and domain boundaries, and extrinsic defects such as foreign atom dopants are identified. Single vacancies are formed by atom ejection and contain dangling bonds. The Stone-Wales defect has a rotated a Ti-O-Ti unit that transforms the hexagonal lattice into nonhexagons. The closed-loops and domain boundaries are constructed from periodic combinations of nonhexagonal rings, such as pentagon-heptagon (5-7) pairs. Ti_2O_3 films exhibit the ability to rearrange the lattice around the intrinsic defects, which changes the electrical and chemical properties of the films. We unravel a substrate-mediated mechanism for the defect formation through enforcing epitaxial strain and tuning adhesion strength of the oxide monolayers. Furthermore, the interactions of extrinsic defects such as foreign atoms (Fe, Nb) can be studied through varying the impurity concentration. Dopant interactions are an important issue for designing the structures and properties of ultrathin oxide films.

Figure. An STM image and a schematic of a closed-loop defect in monolayers of Ti_2O_3 supported on Au(111).



References:
[1] Wu, C.; Castell, M. R.; Goniakowski, J.; Noguera, C. Phys. Rev. B **91**, 155424 (2015).