Electronic Supplementary Material (ESI) for RSC Advances.

Energetics and optical properties of carbon impurities in rutile TiO_2

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A. Chemical potential diagram for equilibrium growth of TiO_2

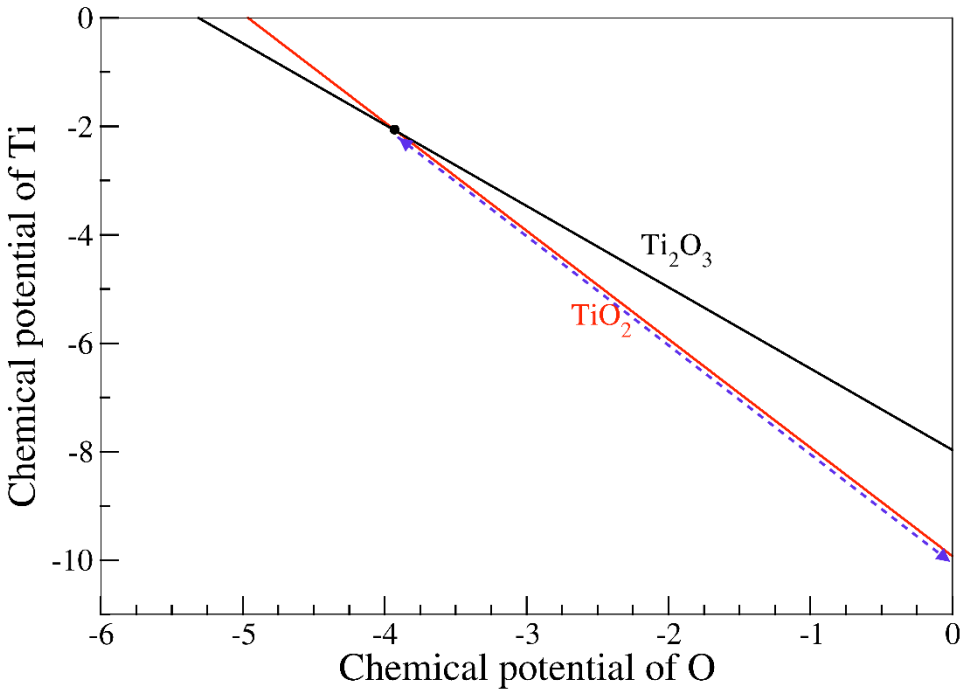

Figure S1. Chemical potential diagram associated with equilibrium growth of TiO_2. For stable growth of TiO_2, the chemical potentials of Ti and O lying on the dashed line are required.

B. Crystal structure, band structure and Brillouin zone of rutile TiO_2

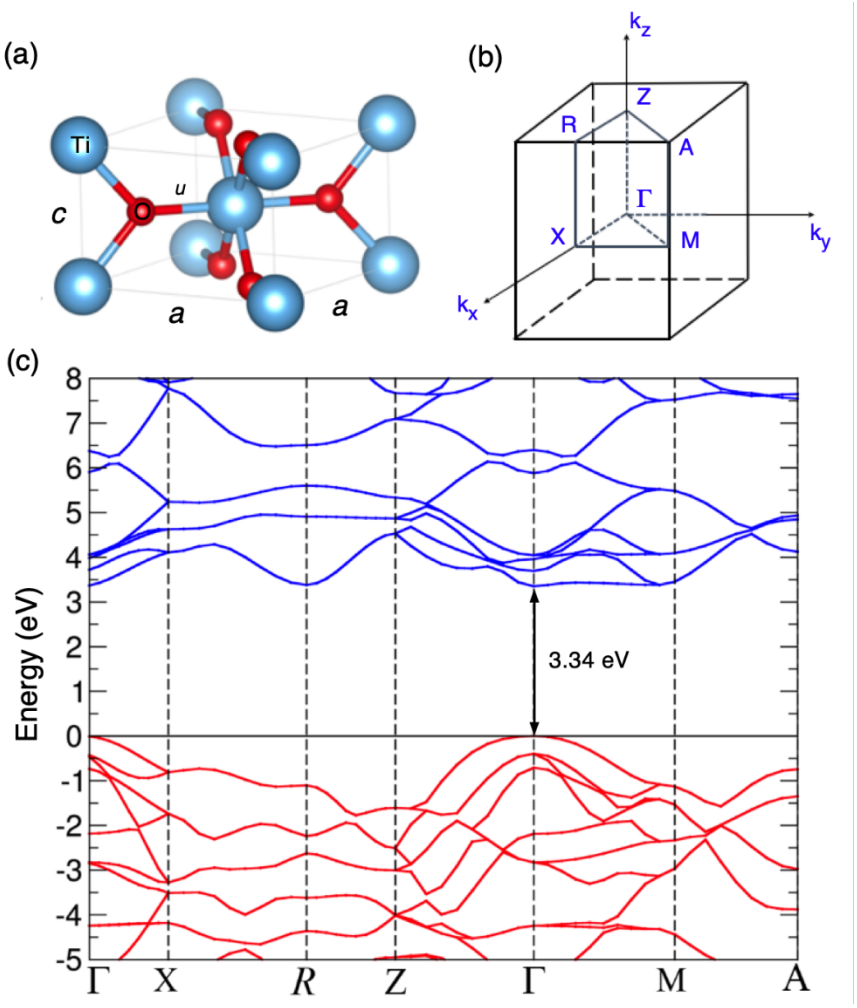

Figure S2 (a) Crystal structure and lattice parameters of rutile TiO_2. (b) The corresponding Brillouin zone. (c) The calculated electronic band structure using HSE functional.

C. Density of states for the substitutional C on O site (C_O)

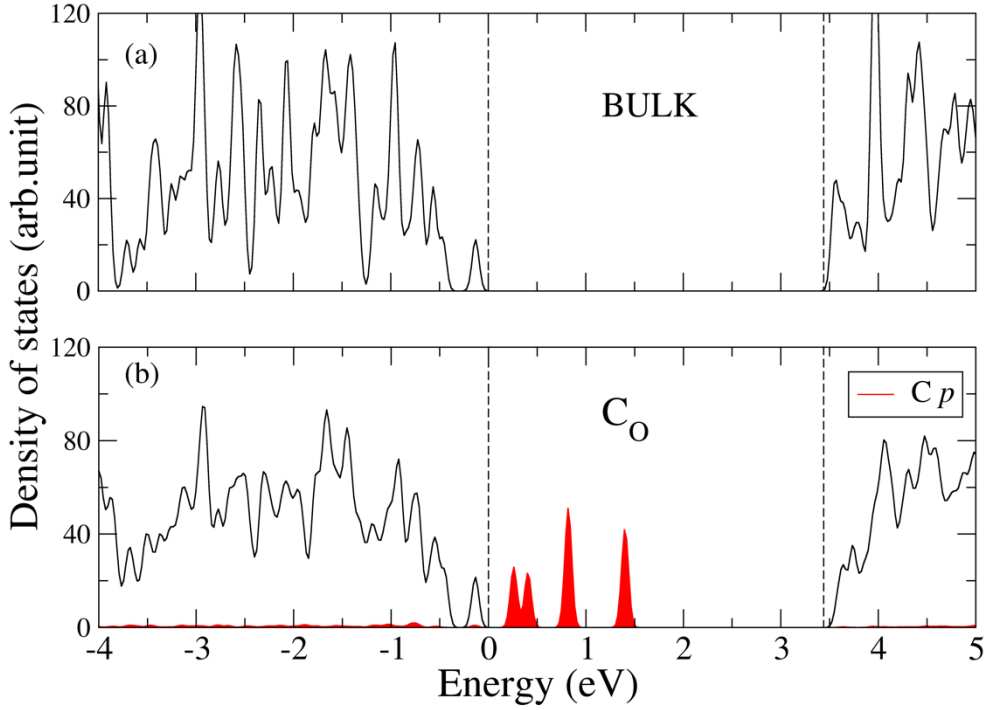

Figure S3 Calculated density of states for (a) defect-free 72-atom atom supercell of rutile TiO2 and (b) the same supercell containing C_O in 2- charge state. The C 2p states are shown as the shaded area with 10 times multiplication of original projected DOS on the C atom for clarity. The dashed lines indicate valence band and conduction edges.