Structural information of the surfaces

Figure S1 show a representation of the unit cell and surface models used in the computational simulations.

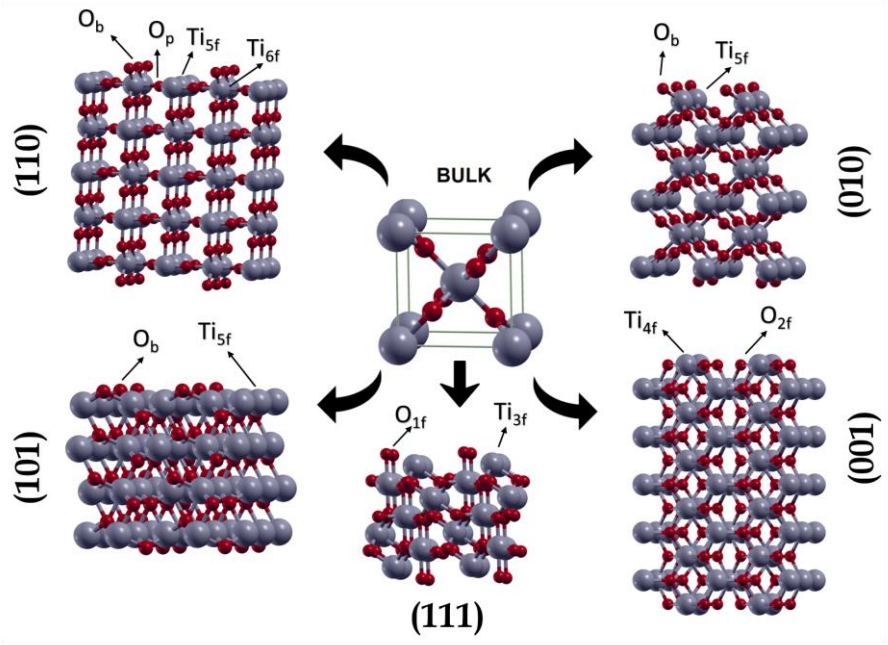

Figure S1 - Bulk and (001), (010), (101), (110) and (111) surface models.

As the surfaces have different kind of slabs with different atoms, the surfaces were modeled with different thickness in the z-direction but were periodic in the x- and y-directions. The surfaces convergences were obtained with a number of 18, 11, 12, 15 and 15 slabs to (100), (001), (101), (110) and (111), respectively. In the Figure S1 were also pointed the atomic sites of the surfaces: O bridge (O_b), O in-plane (O_p), O one-fold (O_{1f}), Ti two-fold (Ti_{2f}), Ti three-fold (Ti_{3f}), Ti four-fold (Ti_{4f}), Ti five-fold (Ti_{5f}) and Ti six-fold (Ti_{6f}).

The results of Mulliken charges for the (110), (010), (101), (001) Surface are listed in the Table S1.

Table S1 - Mulliken charges (in m|e|), for the (110), (010), (101) and (001) Surface Systems.

	Surfaces			
	(110)	(010)	(101)	(001)
O_b	-1.108	-1.171	-	-
O_{2f}	-	-	-	-1.278
O_p	-1.379	-	-1.202	-
Ti_{4f}	-	-	-	2.504
Ti_{5f}	2.619	2.577	2.584	2.504
Ti_{6f}	2.627	-	-	-