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SUPPLEMENTARY FILE

Supplementary Material

Structure and New Substructure of α-Ti_2O_3: X-ray diffraction and Theoretical Study

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Captions:

Table S1: *Atomic coordinates and equivalent isotropic displacement parameters (Å²) for α-Ti_2O_3 (150 K), α-Ti_2O_3 (293 K) and α-Ti_2O_3 substructure (293 K)*
Table S2: *Anisotropic displacement parameters for α-Ti_2O_3 (150 K), α-Ti_2O_3 (293 K) and α-Ti_2O_3 substructure (293 K)*
Table S3: *Selected bond distances (Å) and Bond valence calculation (BVS) for α-Ti_2O_3 (150 K), α-Ti_2O_3 (293 K) and α-Ti_2O_3 substructure (293 K)*

Figure S1: *Typical SEM-EDS spectra obtained on single crystals of the α-Ti_2O_3 samples*
Figure S2: *The group-subgroup relationship between: the structure of the α-Ti_2O_3, the α-Ti_2O_3 substructure and $LiInTi_2O_6$ structure. The indices for the translationengleiche (t) transition and the site symmetries of the Wyckoff sites are given*
Figure S3: *Partial DOS of: (a) α-Ti_2O_3; (b) α-Ti_2O_3 substructure*

Table S1: *Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for α-Ti_2O_3 (150 K), α-Ti_2O_3 (293 K) and α-Ti_2O_3 substructure (293 K)*

	Atoms	*Position*	*x/a*	*y/b*	*z/c*	U_{eq}	*s.o.f*
α-Ti_2O_3 (150 K)	Ti	12c	0	0	0.34448(2)	0.00126(18)	0.97(2)
	O	18e	0.0197(5)	-0.33333	0.416667	0.0047(5)	1
α-Ti_2O_3 (293 K)	Ti	12c	0	0	0.344675(11)	0.00347(8)	0.975(7)
	O	18e	0.31317(11)	0	0.25	0.00449(17)	1
α-Ti_2O_3-sub	Ti	6c	2/3	1/3	0.02266(2)	0.00351(8)	1
(293 K)	O	18g	1/3	0.3537(3)	1/6	0.0052(3)	0.516(8)

U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensors.

Table S2: *Anisotropic displacement parameters for α-Ti_2O_3 (150 K), α-Ti_2O_3 (293 K) and α-Ti_2O_3 substructure (293 K)*

	Atoms	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
α-Ti_2O_3 (150 K)	Ti	0.0008(2)	0.0008(2)	0.0021(3)	0.00042(12)	0	0
	O	0.0024(8)	0.0036(10)	0.0026(8)	0.0018(5)	0.0002(3)	0.0004(6)
α-Ti_2O_3 (293 K)	Ti	0.00358(10)	0.00358(10)	0.00325(11)	0.00179(5)	0	0
	O	0.0048(2)	0.0056(2)	0.0048(2)	0.00282(12)	0.00052(6)	0.00104(3)
α-Ti_2O_3-sub	Ti	0.00367(11)	0.00367(11)	0.00318(12)	0.00184(6)	0	0
(293 K)	O	0.0062(5)	0.0052(4)	0.0046(4)	0.0031(3)	0.0007(3)	0.00036(14)

Table S3: *Selected bond distances (Å) and Bond valence calculation (BVS) for α-Ti_2O_3 (150 K), α-Ti_2O_3 (293 K) and α-Ti_2O_3 substructure (293 K)*

		Distances (Å)	BVS		Distances (Å)
α-Ti_2O_3 (150 K)	Ti-O (x3)	2.0271(13)	0.563 (x3)	Ti-Ti (x1)	2.5668(10)
	Ti-O (x3)	2.0661(16)	0.507 (x3)	Ti-Ti (x4)	2.9963(13)
	BVS		3.715		
α-Ti_2O_3 (293 K)	Ti-O (x3)	2.0739(5)	0.547 (x3)	Ti-Ti (x1)	2.5851(5)
	Ti-O (x3)	2.0340(4)	0.552 (x3)	Ti-Ti (x4)	3.0060(7)
	BVS		3.297		
α-Ti_2O_3-sub	Ti-O (x6)	2.0347(14)	0.551 (x3)	Ti-Ti (x1)	2.5847(7)
(293 K)	Ti-O (x6)	2.0729(11)	0.497 (x3)	Ti-Ti (x4)	3.0060(7)
	BVS		3.146		

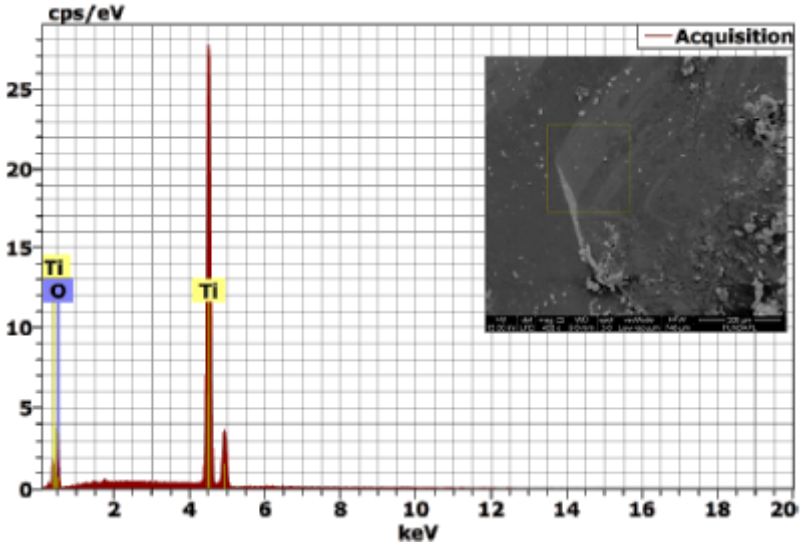
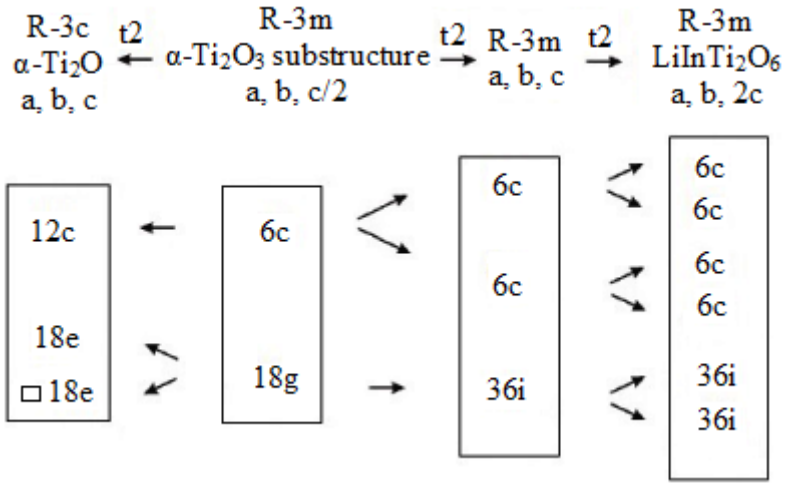


Figure S1: *Typical SEM-EDS spectra obtained on single crystals of the α-Ti_2O_3 samples*



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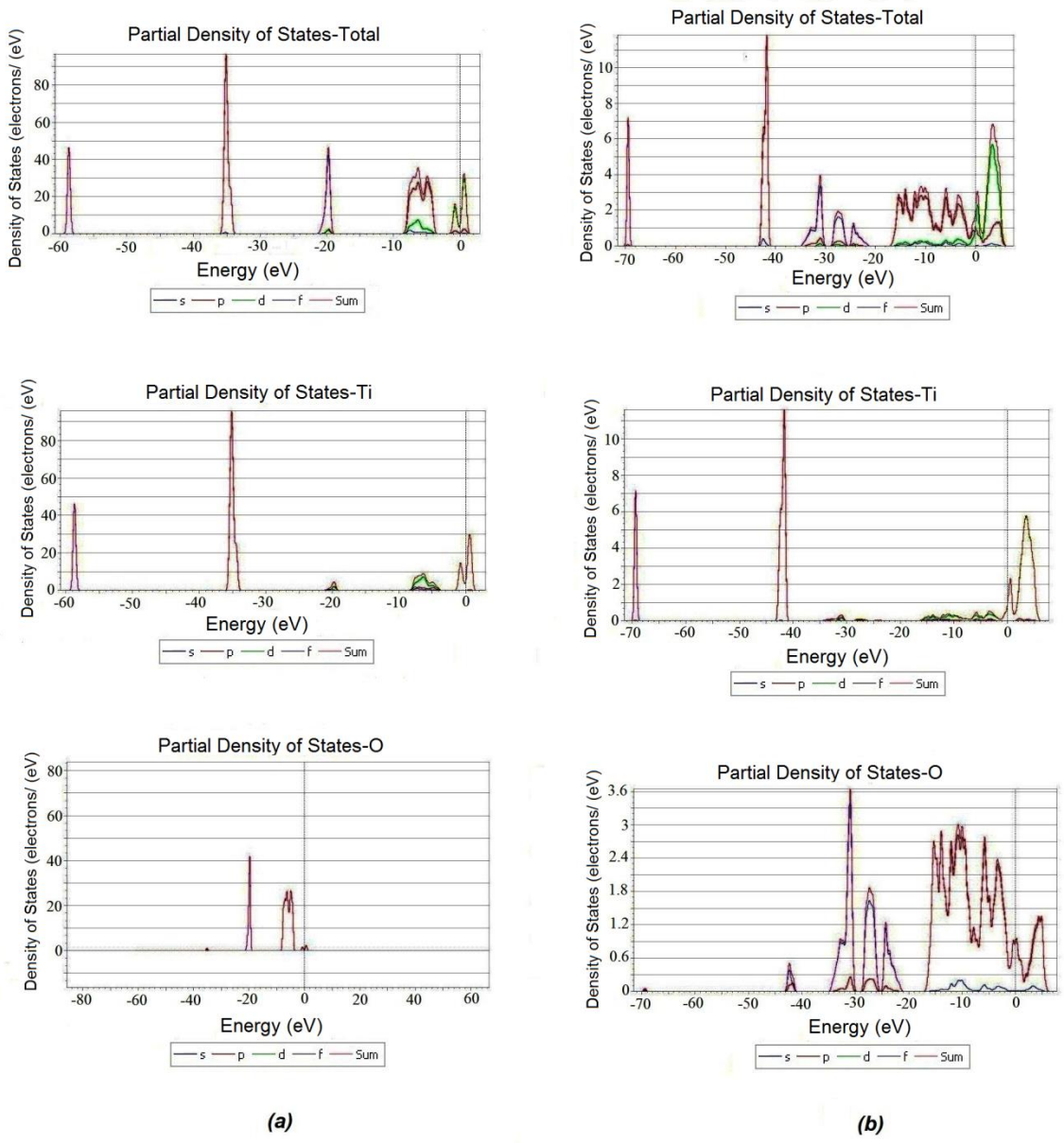

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