

Electronic Supporting Information

Unveiling point defects in titania mesocrystals: a combined EPR and XPS study

Elizaveta Konstantinova^{1,2,3*}, Anton Minnekhanov², Artemii Bulyukov⁴, Vladimir Ivanov^{5,6}, Andrew J. Sutherland⁷ and Olga Boytsova^{5,6*}

¹Department of Physics, Lomonosov Moscow State University, Leninskie Gory 1-2, 119991 Moscow, Russia

²National Research Center Kurchatov Institute, Kurchatov Square 1, 123182 Moscow, Russia

³Department of Nano-, Bio-, Information Technology and Cognitive Science, 141701 Dolgoprudny, Moscow Region, Russia

⁴Physical-Technical Institute of UB RAS, Kirova Str. 132, 426000 Izhevsk, Russia

⁵Kurnakov Institute of General and Inorganic Chemistry Russian Academy of Sciences, Leninskii Ave. 31, 119991 Moscow, Russia

⁶Department of Materials Science, Lomonosov Moscow State University, Leninskie Gory 1-3, 119991 Moscow, Russia

⁷Aston Institute of Materials Research, Aston University, Aston Triangle, Birmingham, B4 7ET, UK.

Content	Page
Table of Contents	S1
XRD patterns of Ti-based mesocrystals	S2
XPS data	S3
Representative full isotherm of N ₂ adsorption	S4

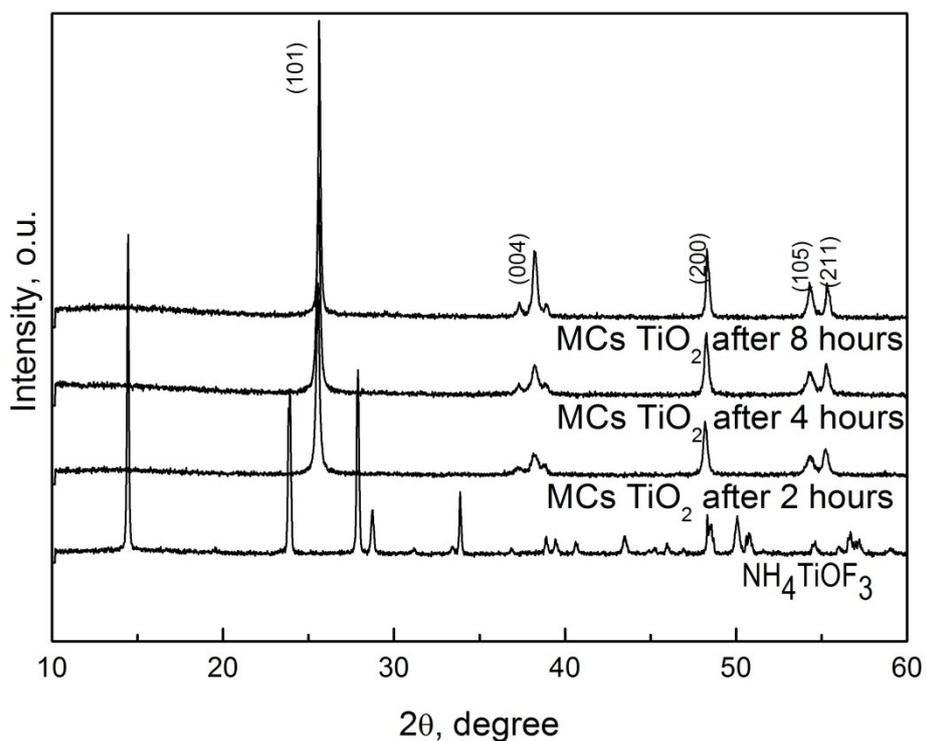


Figure S1 XRD patterns of the first formed NH_4TiOF_3 MCs and the TiO_2 MCs formed from the thermally-mediated transformation of NH_4TiOF_3 MCs after 2, 4 and 8 hours of annealing. (Data reproduced from O. V. Boytsova, A. A. Sadovnikov, K. E. Yorov, A. N. Beltiukov, A. E. Baranchikov, V. K. Ivanov, X. Zhong, D. J. Lewis, P. O'Brien and A. J. Sutherland, *CrystEngComm.*, 2017, **19**, 3281.)¹¹

Table 1 Atomic concentration of components of MCs from XPS (Data reproduced from O. V. Boytsova, A. A. Sadovnikov, K. E. Yorov, A. N. Beltiukov, A. E. Baranchikov, V. K. Ivanov, X. Zhong, D. J. Lewis, P. O'Brien and A. J. Sutherland, *CrystEngComm.*, 2017, **19**, 3281.)¹¹

Sample	Ti	O	C	F	K	C/Ti	F/Ti
NH ₄ TiOF ₃ MCs	11.88	23.32	12.45	41.7	0.75	1.05	3.5
TiO ₂ MCs (2 h anneal)	20.72	53.54	11.65	8.98	5.11	0.56	0.43
TiO ₂ MCs (4 h anneal)	21.71	54.87	8.40	10.37	4.65	0.39	0.48
TiO ₂ MCs (8 h anneal)	21.60	55.87	8.47	9.33	4.73	0.39	0.43

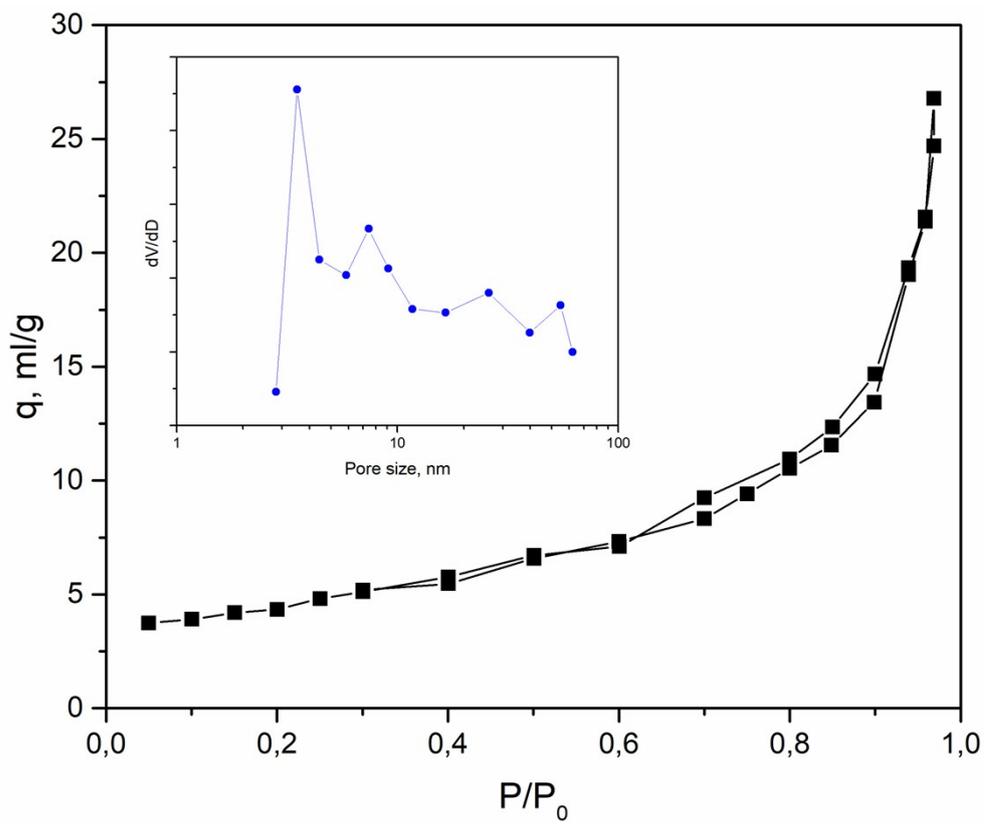


Figure S2 Representative full N₂ isotherm for TiO₂ MCs after 2 h anneal.