

Supplementary information: The Cerium/Boron Insertion Impact in Anatase Nano-structures on the Photoelectrochemical and Photocatalytic response

A. A. Flores-Caballero ^{1, 2}, A. Manzo-Robledo ¹ and N. Alonso-Vante ^{2,*}

Section 1: XRD and SEM





Citation: Flores-Caballero, A.A.; Manzo-Robledo, A.; Alonso-Vante, N. The Cerium/Boron Insertion Impact in Anatase Nano-structures on the Photo-electrochemical and Photocatalytic response. *Surfaces* **2021**, *4*, 54–65. https://doi.org/ 10.3390/surfaces4010008

Academic editor: Gaetano Granozzi Received: 23 December 2020 Accepted: 2 February 2021 Published: 15 February 2021

Publisher's Note: MDPI stays neutral with regard to jurisdictional claims in published maps and institutional affiliations.



Copyright: © 2021 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses /by/4.0/).

Sample	a / Å (error)	c / Å (error)	< d > / nm (error)	ε/ microstrain	Unit Cell volume (ų)
				(error)	
TiO ₂	3.7872 (1.5E-4)	9.5032	14.1 (0.03)	0.0039	136.30
		(4.2E-4)		(2.0E-5)	
TiO ₂ -B	3.7875 (1.6E-4)	9.5038	13.3 (0.03)	0.0040	136.33
		(4.6E-4)		(8.4E-6)	
TiO ₂ -Ce	3.7942 (2.0E-4)	9.5105	11.4 (0.03)	0.0046	136.91
		(5.8E-4)		(2.5E-5)	

Table S1. Structural properties from Rietvel analysis for TiO2, TiO2-B and TiO2-Ce samples (cf. Figure S1(b)).



Figure S2. SEM morphologies of P25, TiO₂, B and Ce-doped anatase.

Section 2: XPS Survey



Figure S3. XPS general spectra of TiO_2 nanoparticles modified with boron and cerium: TiO_2 -B and TiO_2 -Ce.

Species		TiO ₂ -B		TiO2-Ce	
		Weight	Bind energy	Weight	Bind energy
		(%)	(eV)	(%)	(eV)
B 1s	B–N	6.59	190.8	-	-
	H ₃ BO ₃	11.44	193.7	-	-
	B–O, BCO ₂	30.6	192.08	-	-
	B_2O_3	51.38	192.85	-	-
O 1s	TiO ₂	85.48	530.03	76.7	529.94
	OH ads	-	-	4.3	532.21
	Carbonates	7.84	531.19	8.6	531.2
	В–О, Ті–О–В,	3.99	532.15	-	-
	Nitrates				
	Al ₂ O ₃	2.3	528.49	-	-
	B ³⁺ (B ₂ O ₃)	0.39	533.07	-	-
	Ce^{4+} (CeO ₂)	-	-	3	528.51
	Ce^{3+} (Ce ₂ O ₃)	-	-	7.5	530.59
Ce 3d _{3/2} , 5/2	Ce ³⁺	-	-	72.8	885.7
	Ce^{4+}	-	-	27.2	882.55
Ti 2p	4) Ti(IV)	73.7	458.71	72.76	458.72
	3) Ti(IV)-Ce	13.4	458.05	13.24	458
	5) TiO(OH)2	4.7	459.85	5	459.85
	2) Ti(III)	4.5	456.99	4.8	457.04
	1) Ti(II)	1.9	456	2.13	456.09
	6) Ti-C	1.9	460.75	2.07	460.75

Table S2. Weight composition of O1s, Ce3d $_{3/2}$, $_{5/2}$ and B1s collected from the modified TiO₂.

Section 3: Cyclic Voltammetry in darkness



Figure S4. Current-potential characteristics of oxides deposited onto SnO₂: F (FTO) in dark in 0.5M H₂SO₄. (a) FTO, (b) TiO₂ anatase, (c) TiO₂-B, and (d) TiO₂-Ce. Scan rate: 50 mV/s.

Section 4: Photoactivity characteristics



Figure S5. Photocurrent-potential characteristics of doped-oxides (TiO₂-B, and TiO₂-Ce). Scan rate: 1 mV/s. The mass deposited on each sample was 0.2 mg/cm^2 .