Carbon-doped anatase titania nanoparticles: similarities and differences with respect to bulk and extended surface models

Elena R. Remesal, Ángel Morales-García*

Departament de Ciència de Materials i Química Física & Institut de Química Teòrica i Computacional (IQTCUB), Universitat de Barcelona, c/ Martí i Franquès 1-11, 08028 Barcelona, Spain

e-mail: angel.morales@ub.edu

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Figures S1 to S3 shows to the sites where take place the doping at oxygen, titanium and interstitial sites, respectively.

Table S1 compiles the formation energy of C-doping at oxygen and titanium sites in the anatase bulk phase.

Table S2 compiles the formation energy of C-doping titania at oxygen, titanium and interstitial sites in the $(TiO_2)_{84}$ NP.

Table S3 compiles the energy gap, and the energy orbitals LUMO (eV) and HOMO (eV) of carbon doping titania using PBE and PBEx density functionals.

Fig. S1 Side and top views of the optimized $(TiO_2)_{84}$ NPs C-doping at O sites (C_O). Blue, red, and black spheres denote titanium, oxygen, and carbon, respectively. Note that C-atom have been represented with double radius to show clearly doping site.

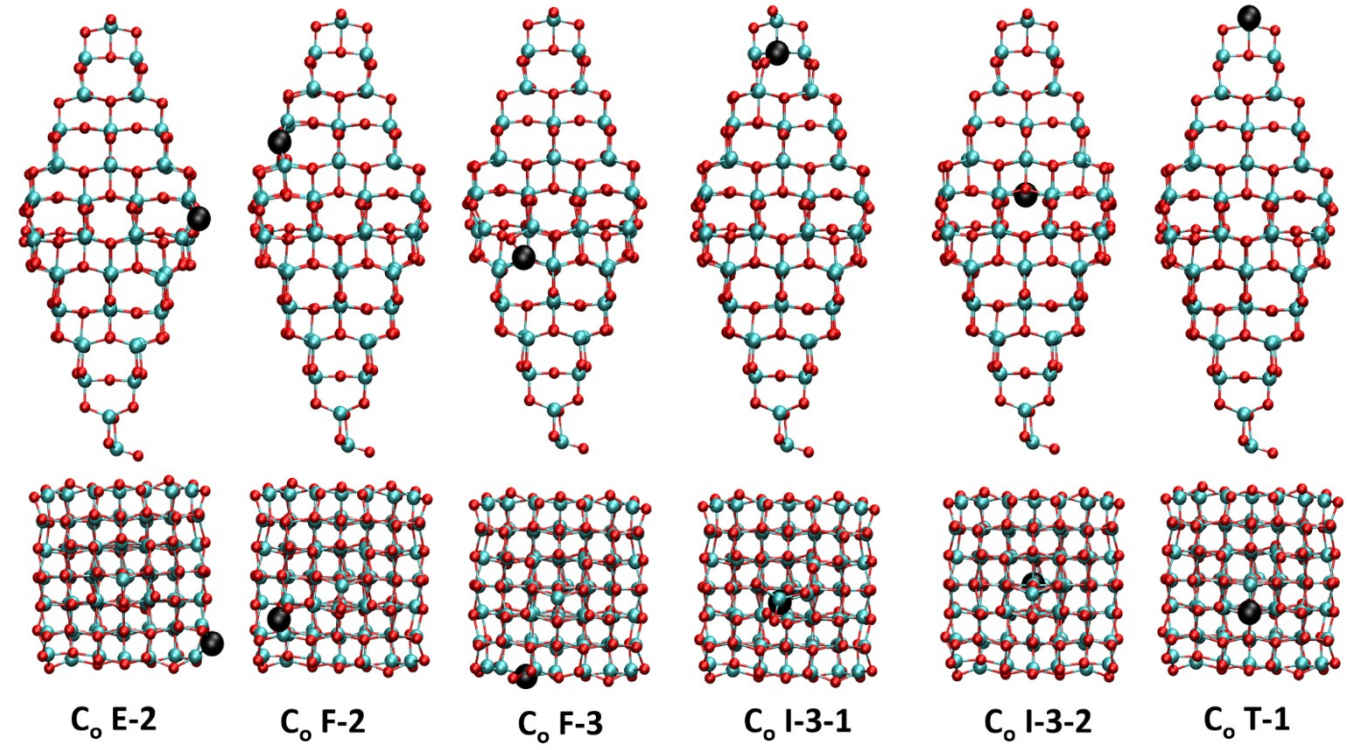

Fig. S2 Side and top views of the optimized $(TiO_2)_{84}$ NPs C-doping at Ti site (C_{Ti}). Blue, red, and black spheres denote titanium, oxygen, and carbon, respectively. Note that C-atom have been represented with double radius to show clearly doping site.

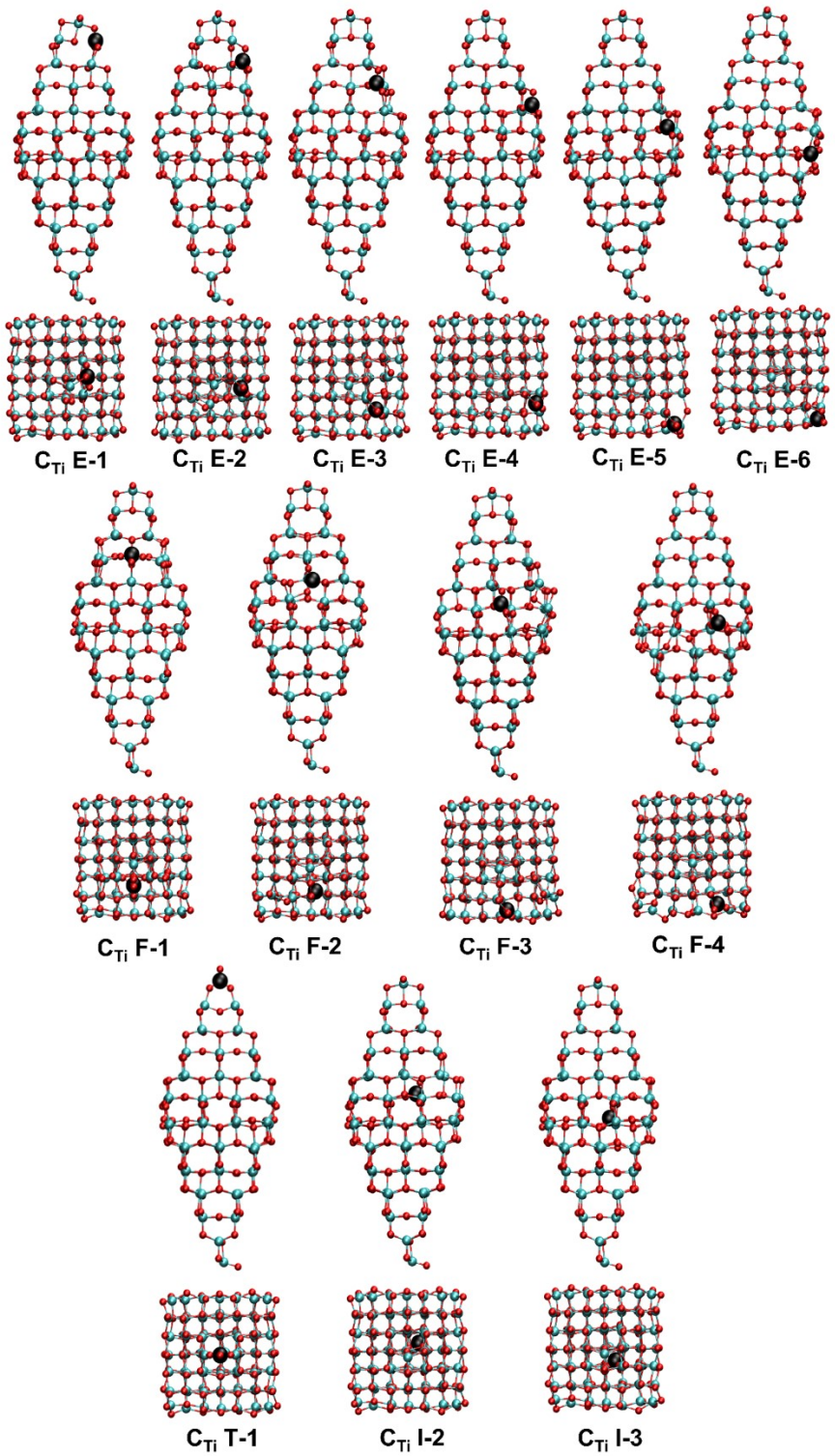

Fig. S3 Side and top views of the different C_i doping $(TiO_2)_{84}$ NPs. Blue, red, and black spheres denote titanium, oxygen, and carbon, respectively. Note that C-atom have been represented with double radius to show clearly doping site.

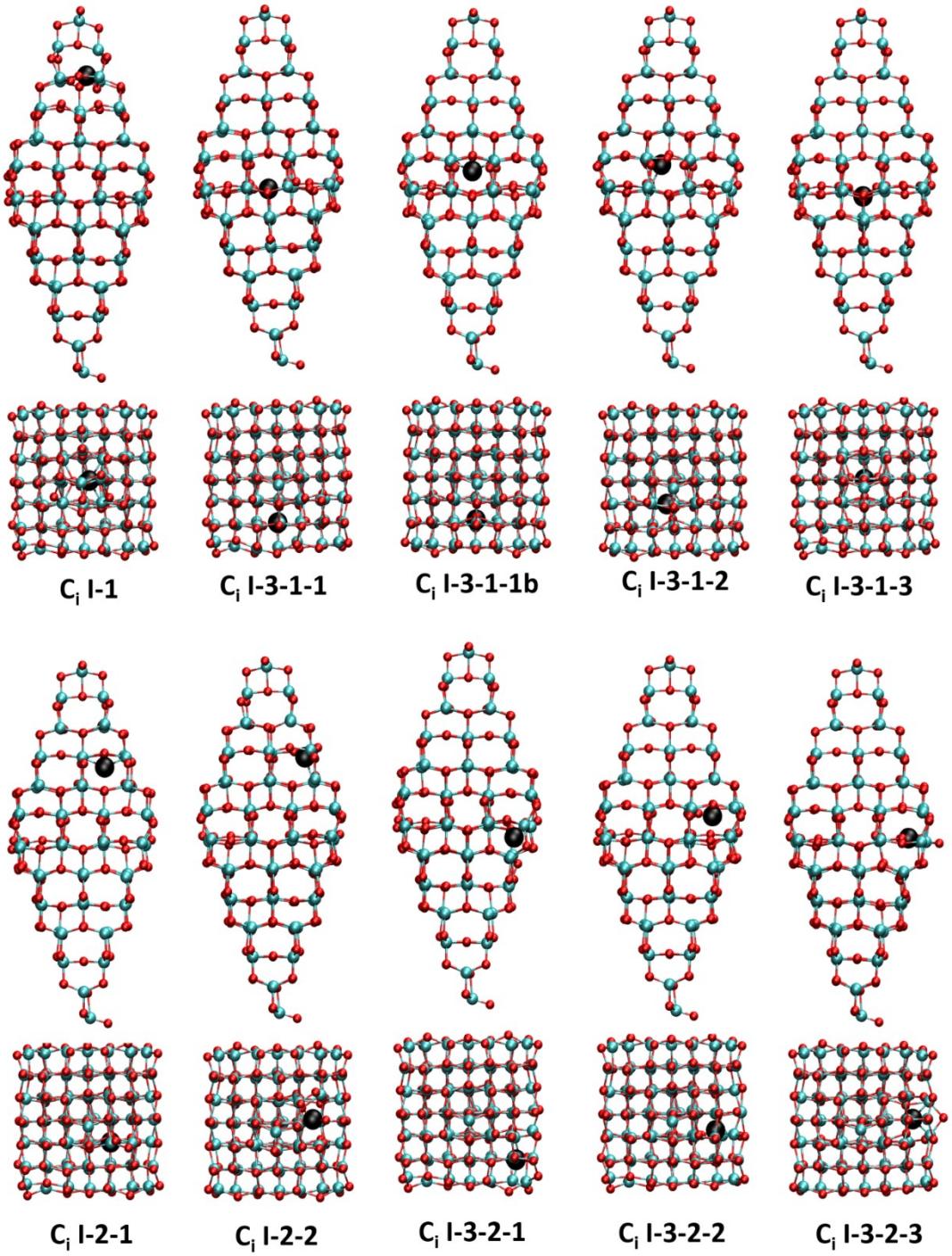

Table S1. Formation energy (in eV) of C-doped anatase bulk system as a function of the oxygen chemical potential (in eV). Formation of C_O and C_{Ti} are included considering the (1x1x1) and the (2x2x2) anatase supercells.

	μ_O'				
	-4	-3	-2	-1	0
1x1x1 C_O- TiO_2	8.38	9.38	10.38	11.38	12.38
1x1x1 C_{Ti}- TiO_2	16.09	14.09	12.09	10.09	8.09
2x2x2 C_O- TiO_2	8.50	9.50	10.50	11.50	12.50
2x2x2 C_{Ti}- TiO_2	17.17	15.17	13.17	11.17	9.17

Table S2. Formation energy (in eV) of C-doped TiO_2 NPs as a function of the oxygen chemical potential (in eV).

NP	μ_O'				
	-4	-3	-2	-1	0
C_O E-2	7.41	8.41	9.41	10.41	11.41
C_O F-2	7.68	8.68	9.68	10.68	11.68
C_O F-3	7.70	8.70	9.70	10.70	11.70
C_O I-3-1	6.60	7.60	8.60	9.60	10.60
C_O I-3-2	8.42	9.42	10.42	11.42	12.42
C_O T-1	9.13	10.13	11.13	12.13	13.13
C_{Ti} T-1	12.40	10.40	8.40	6.40	4.40
C_{Ti} E-1	14.00	12.00	10.00	8.00	6.00
C_{Ti} E-2	12.73	10.73	8.73	6.73	4.73
C_{Ti} E-3	12.97	10.97	8.97	6.97	4.97
C_{Ti} E-4	13.29	11.29	9.29	7.29	5.29
C_{Ti} E-5	13.34	11.34	9.34	7.34	5.34
C_{Ti} E-6	14.61	12.61	10.61	8.61	6.61
C_{Ti} F-1	15.79	13.79	11.79	9.79	7.79
C_{Ti} F-2	14.78	12.78	10.78	8.78	6.78
C_{Ti} F-3	13.90	11.90	9.90	7.90	5.90
C_{Ti} F-4	13.69	11.69	9.69	7.69	5.69
C_{Ti} I-2	13.69	11.69	9.69	7.69	5.69
C_{Ti} I-3	14.85	12.85	10.85	8.85	6.85
C_i I-1	-	-	-	-	8.97
C_i I-2-1	-	-	-	-	9.31
C_i I-2-2	-	-	-	-	8.68
C_i I-3-1-1	-	-	-	-	8.75
C_i I-3-1-1B	-	-	-	-	8.96
C_i I-3-1-2	-	-	-	-	8.25
C_i I-3-1-3	-	-	-	-	9.03
C_i I-3-2-1	-	-	-	-	8.37
C_i I-3-2-2	-	-	-	-	8.36
C_i I-3-2-3	-	-	-	-	8.34

Table S3. Energy gap, LUMO (eV) and HOMO (eV) of C-doped $(TiO_2)_{84}$ NPs described with PBE and PBEx density functionals.

NP	PBE			PBEx		
	Egap	LUMO	HOMO	Egap	LUMO	HOMO
C_O E-2	0.47	-4.89	-5.36	1.14	-4.62	-5.76
C_O F-2	0.27	-4.91	-5.18	0.88	-4.63	-5.51
C_O F-3	0.74	-4.90	-5.65	1.53	-4.62	-6.15
C_O I-3-1	0.94	-4.95	-5.89	1.70	-4.67	-6.37
C_O I-3-2	0.67	-5.58	-6.25	1.13	-5.78	-6.92
C_O T-1	0.68	-4.91	-5.59	0.83	-4.64	-5.47
C_{Ti} T-1	2.07	-4.94	-7.01	3.16	-4.65	-7.81
C_{Ti} E-1	2.20	-4.95	-7.15	-	-	-
C_{Ti} E-2	2.94	-4.50	-7.44	3.58	-4.65	-8.23
C_{Ti} E-3	2.53	-4.90	-7.42	3.61	-4.60	-8.21
C_{Ti} E-4	2.52	-4.89	-7.40	-	-	-
C_{Ti} E-5	2.54	-4.90	-7.44	-	-	-
C_{Ti} E-6	2.32	-4.93	-7.26	-	-	-
C_{Ti} F-1	2.46	-4.90	-7.36	-	-	-
C_{Ti} F-2	2.45	-4.93	-7.38	-	-	-
C_{Ti} F-3	2.49	-4.91	-7.40	-	-	-
C_{Ti} F-4	2.37	-4.95	-7.32	-	-	-
C_{Ti} I-2	2.51	-4.86	-7.37	-	-	-
C_{Ti} I-3	2.56	-4.86	-7.42	-	-	-
C_i I-1	1.42	-4.95	-6.37	-	-	-
C_i I-2-1	1.38	-4.90	-6.29	-	-	-
C_i I-2-2	0.49	-4.94	-5.42	-	-	-
C_i I-3-1-1	0.04	-4.82	-4.86	-	-	-
C_i I-3-1-1b	1.03	-4.90	-5.94	-	-	-
C_i I-3-1-2	0.11	-4.97	-5.08	0.22	-4.58	-4.79
C_i I-3-1-3	0.05	-4.81	-4.85	-	-	-
C_i I-3-2-1	1.33	-4.91	-6.24	-	-	-
C_i I-3-2-2	0.08	-4.81	-4.89	-	-	-
C_i I-3-2-3	0.25	-4.91	-5.16	0.92	-4.63	-5.55