

***In Situ* Growth of Bi Nanoparticles on NaBiO₃, δ-, and β-Bi₂O₃ Surfaces: Electron Irradiation and Theoretical Insights**

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Supporting Information

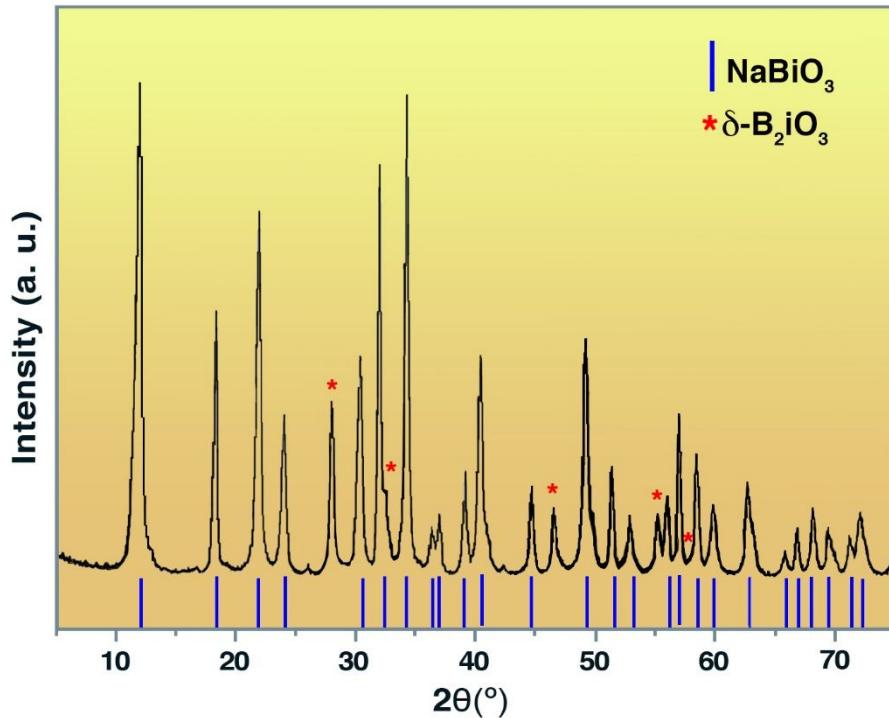


Figure S1– XRD patterns for commercial NaBiO₃.

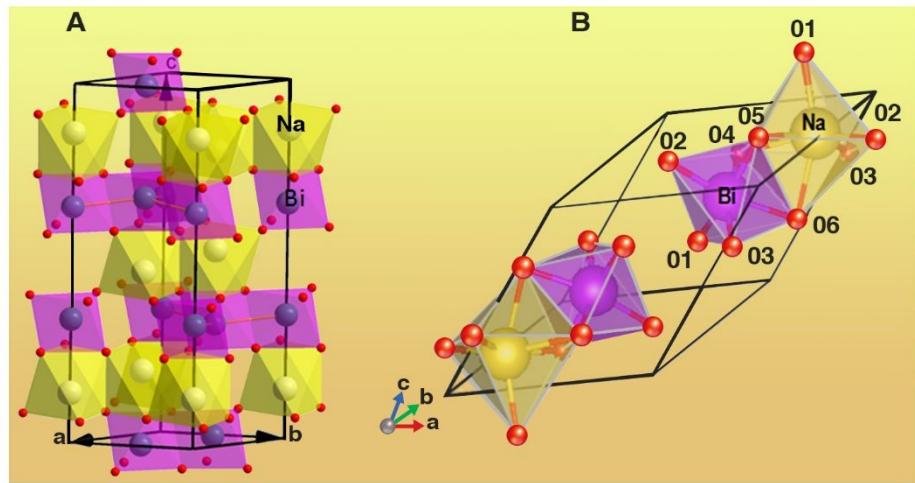


Figure S2– Conventional (A) and primitive cell (B) of NaBiO_3 in the rhombohedral space group R-3

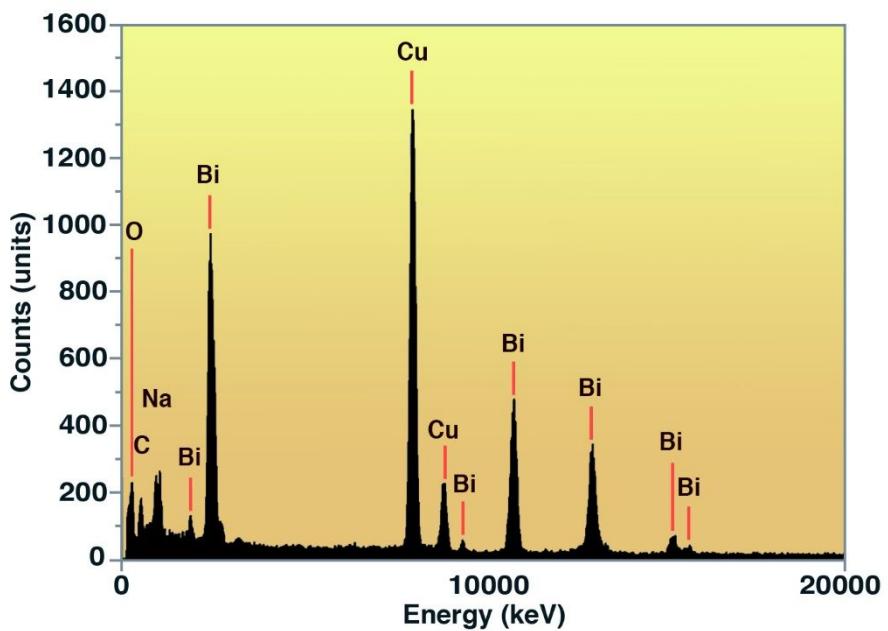


Figure S3– EDS analysis of NaBiO_3 .

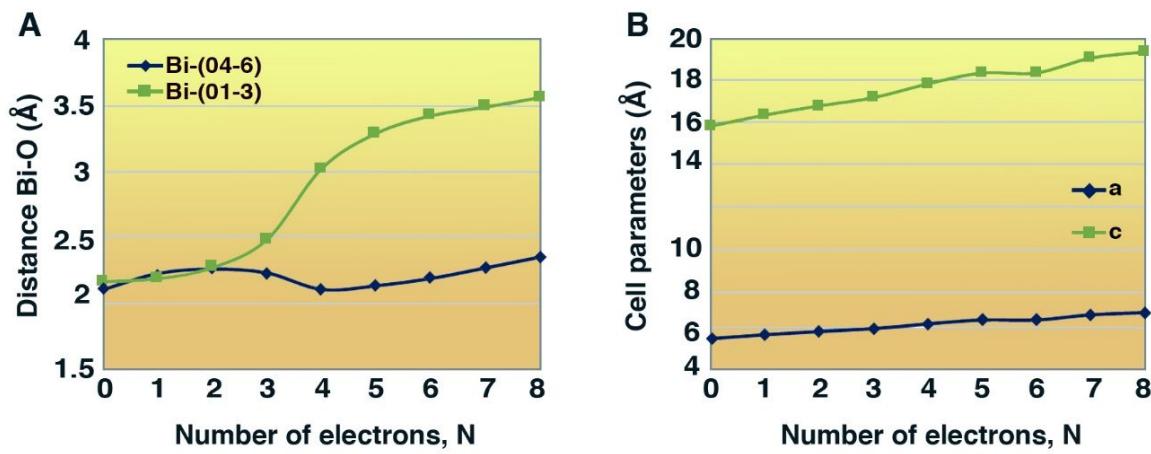


Figure S4 – (A) Variation of Bi-O distances (B) and of cell parameters in NaBiO_3 structure as a function of the number of electrons added, N.

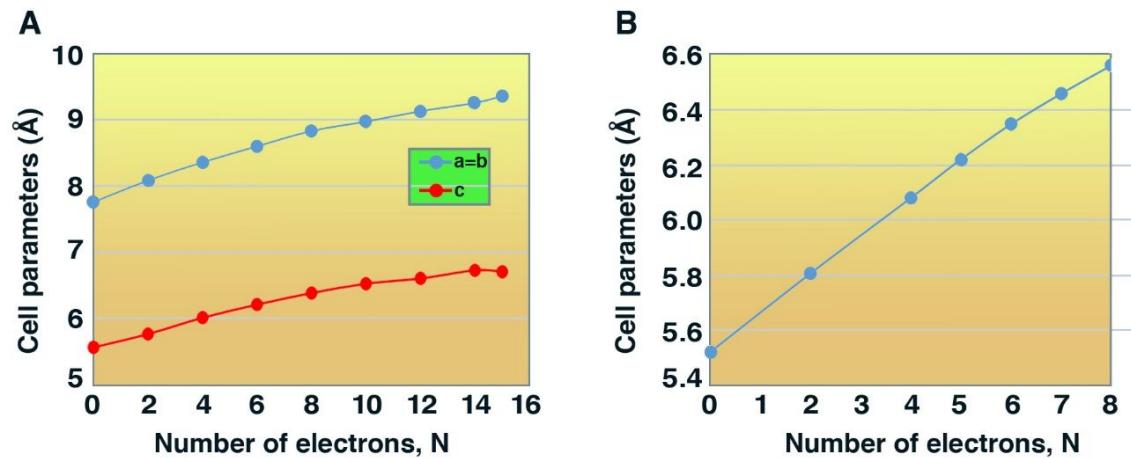


Figure S5 – (A) Variation of cell parameters in $\beta\text{-Bi}_2\text{O}_3$ structure as a function of the number of electrons added, N. (B) $\delta\text{-Bi}_2\text{O}_3$.

Table S1 -Values of charge density for Na, Bi and O centers in NaBiO₃ structure as a function of the number of electrons added, N.

N	Na	Bi	O
0	0,8695	2,3701	-1,0799
1	0,8632	2,1218	-1,1617
2	0,8524	1,9240	-1,2588
3	0,8395	1,6839	-1,3411
4	0,8310	1,3826	-1,4045
5	0,8169	1,0191	-1,4453
6	0,8053	0,6780	-1,4944
7	0,7969	0,3188	-1,5386
8	0,7545	-0,0068	-1,5621

Table S2 -Values of charge density for Na, Bi and O centers in β-Bi₂O₃ and δ-Bi₂O₃ structures as a function of the number of electrons added, N.

N e	β-Bi ₂ O ₃		δ-Bi ₂ O ₃	
	Bi	O	Bi	O
0	1,7692	-1,2001	1,7701	-1,2369
2	1,5689	-1,2303	1,3607	-1,2983
4	1,3599	-1,2506	0,9338	-1,3399
6	1,1282	-1,2630	0,4728	-1,3620
8	0,8837	-1,2695	0,0573	-1,4042
10	0,6367	-1,2707		
12	0,4052	-1,2820		
14	0,1788	-1,2938		
15	0,0313	-1,2758		