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Supplementary Information

Combined Experimental-Theoretical Study of the Optoelectronic Properties of Non-Stoichiometric Pyrochlore Bismuth Titanate

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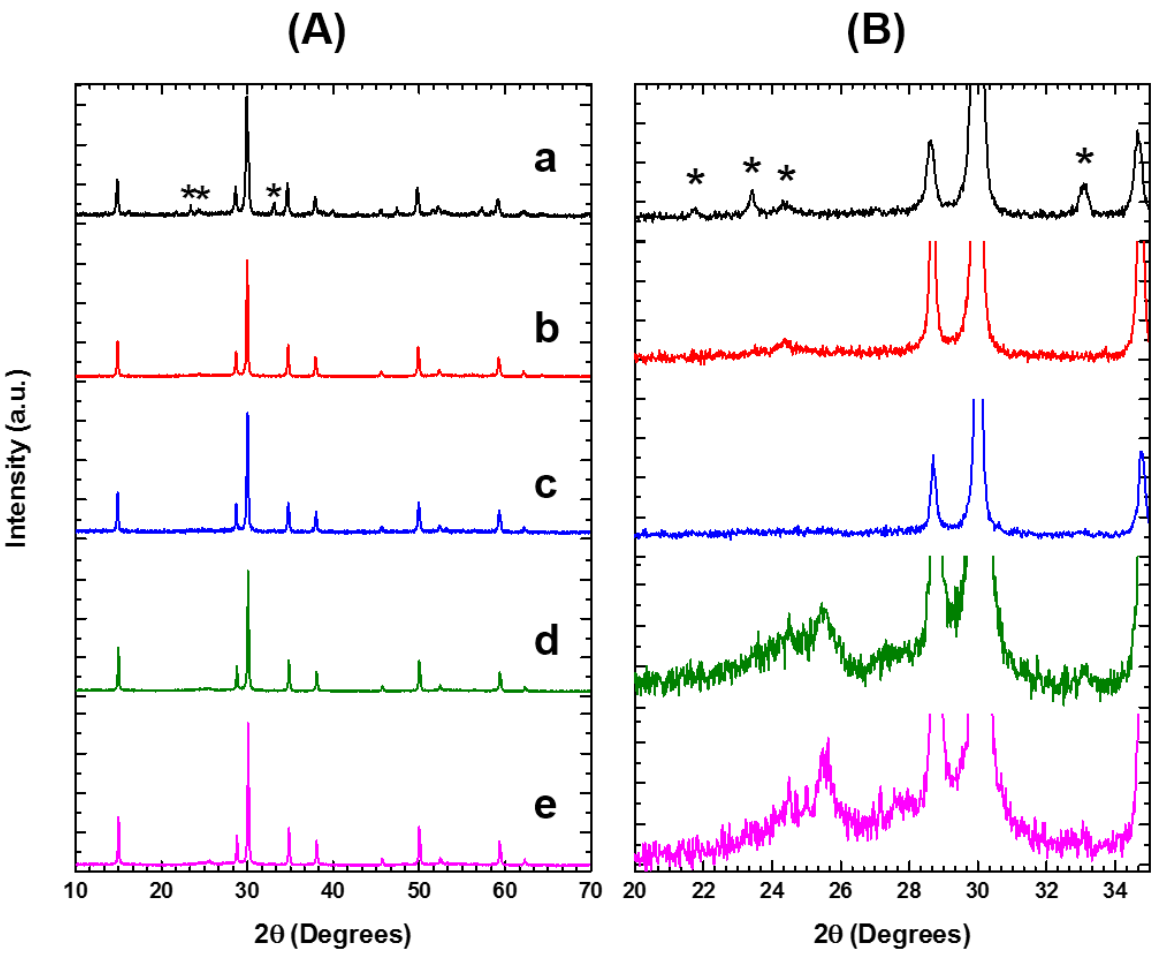

Fig. S1. A) XRD patterns of the powder samples prepared with different Ti/Bi ratio of (a) 1, b) 1.23, c) 1.50, d) 1.75, e) 2.00. B) The magnified XRD patterns where the amorphous phases and the $Bi_4Ti_3O_{12}$ secondary phase (asterisk) are observed.

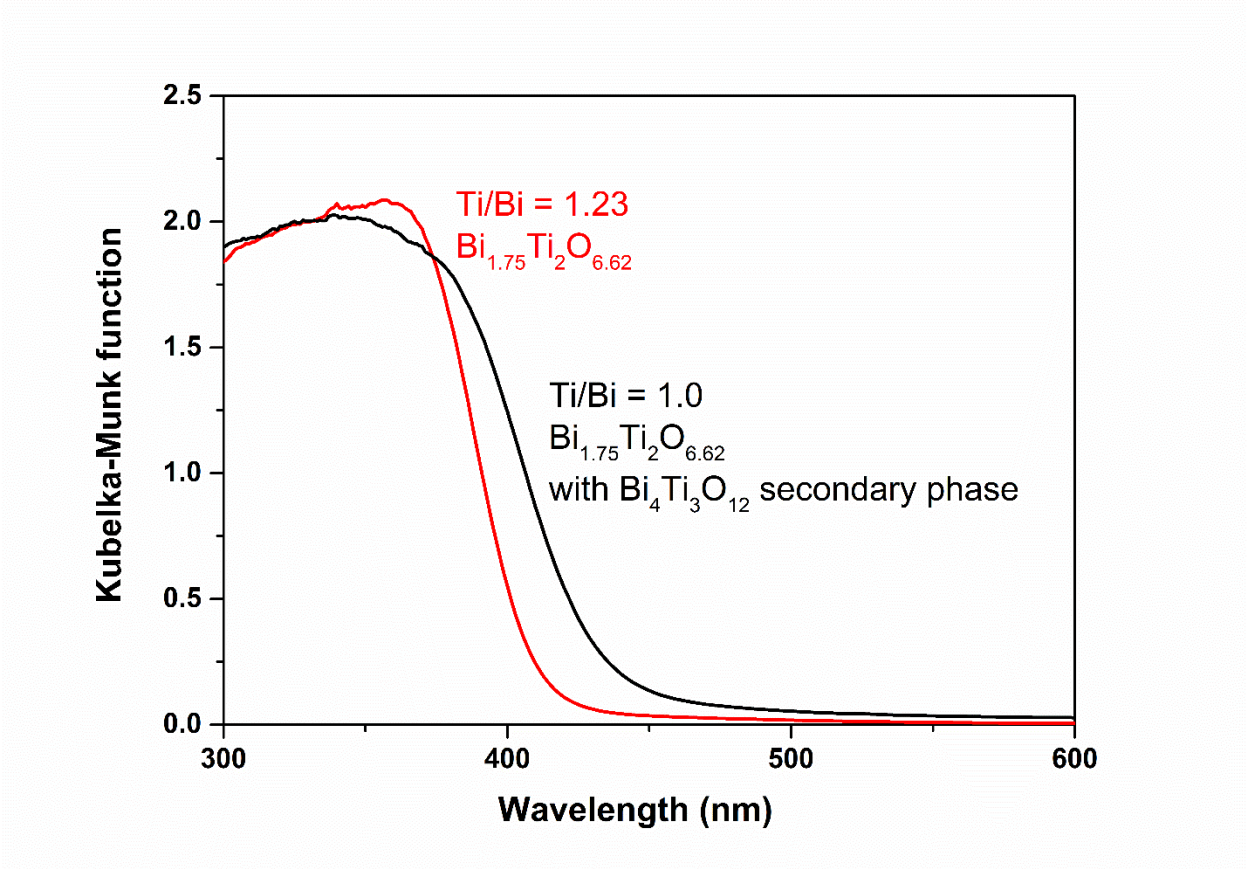

Fig. S2. Diffuse reflectance UV-Vis spectra of the powder sample with Ti/Bi = 1.0 containing $Bi_4Ti_3O_{12}$ secondary phase and the sample with Ti/Bi = 1.23 (single phase).

Table S1. Rietveld atomic positions and occupancy for bismuth, titanium, and oxygen atoms in $Bi_{1.75}Ti_2O_{6.62}$ sample.

atom	**Wyckoff position**	**x**	**y**	**z**	**occupancy**
Bi	96	0.00000	-0.02846	0.02846	0.1463
Ti	16	0.50000	0.50000	0.50000	1
O	48	0.12500	0.12500	0.43297	1
O’	8	0.12500	0.12500	0.12500	0.624

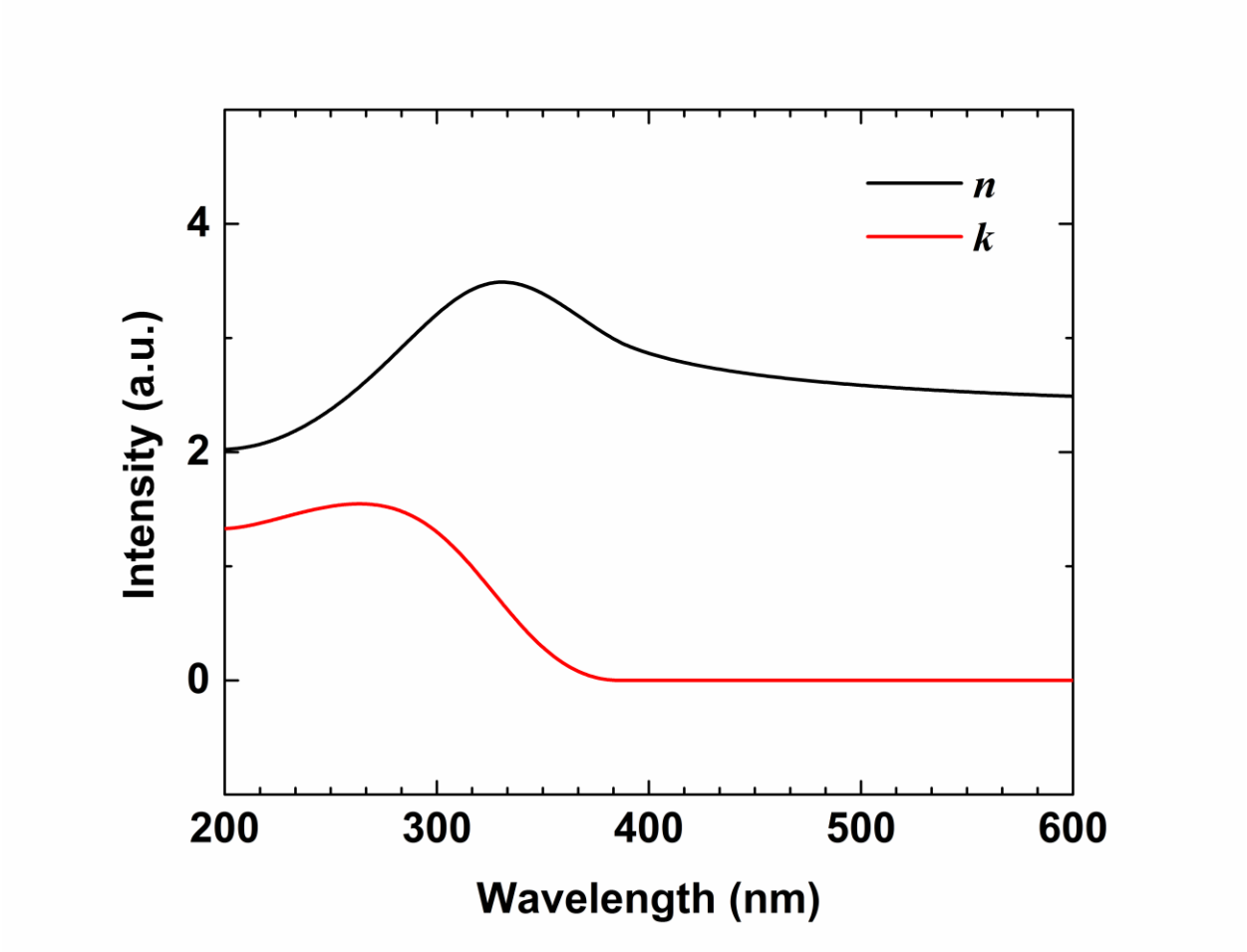

Fig. S3. Refractive index components measured by spectroscopic ellipsometry for $Bi_{1.75}Ti_2O_{6.62}$/Si film.

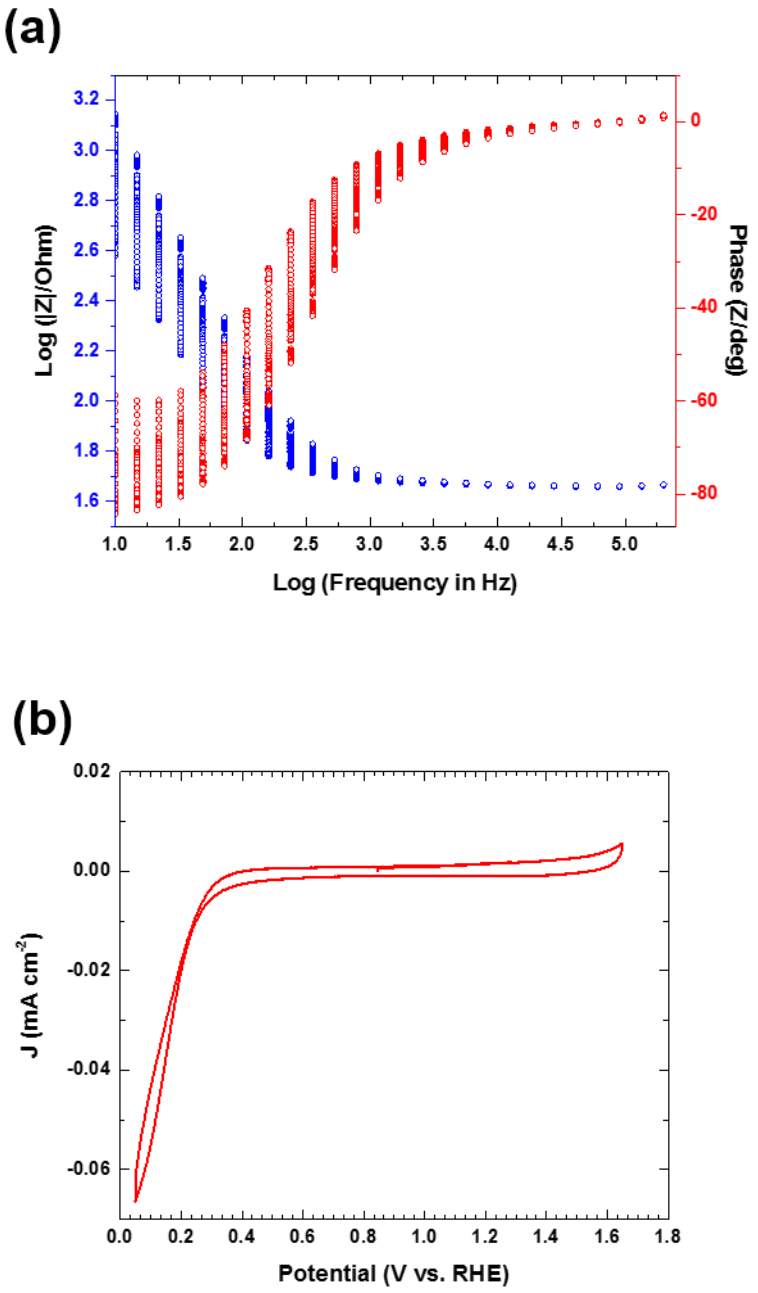

Fig. S4. a) Cyclic voltammetry $Bi_{1.75}Ti_2O_{6.62}$/FTO film measured in 0.1 M NaOH solution, pH 13, b) the XRD of the $Bi_{1.75}Ti_2O_{6.62}$/FTO film used for Mott-Schottky (stars correspond to peaks of FTO substrate).