Supplementary Materials

Structural and Optical Properties of Ba3(Nb6-xTax)Si4O26 (*x*=0.6, 1.8, 3.0, 4.2, 5.4)

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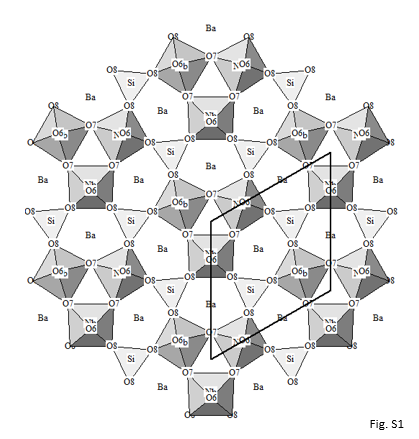


Fig. S1. [001] projection of the crystal structure of Ba3(Nb6-xTax)Si4O26 derived from the X-ray powder data, showing cornered-shared (Ta,Nb)O6 octahedra and SiO4 tetrahedra. Atomic labeling are shown.

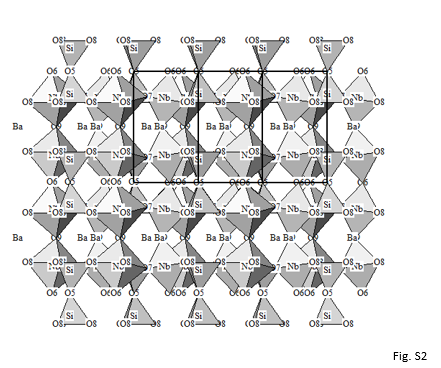


Fig. S2. [110] projection of the crystal structure of Ba3(Nb6-xTax)Si4O26 showing the Ba-filled distorted 5-fold coordination channels. Atomic labeling are shown.

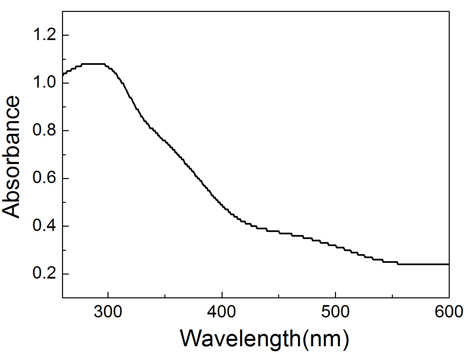
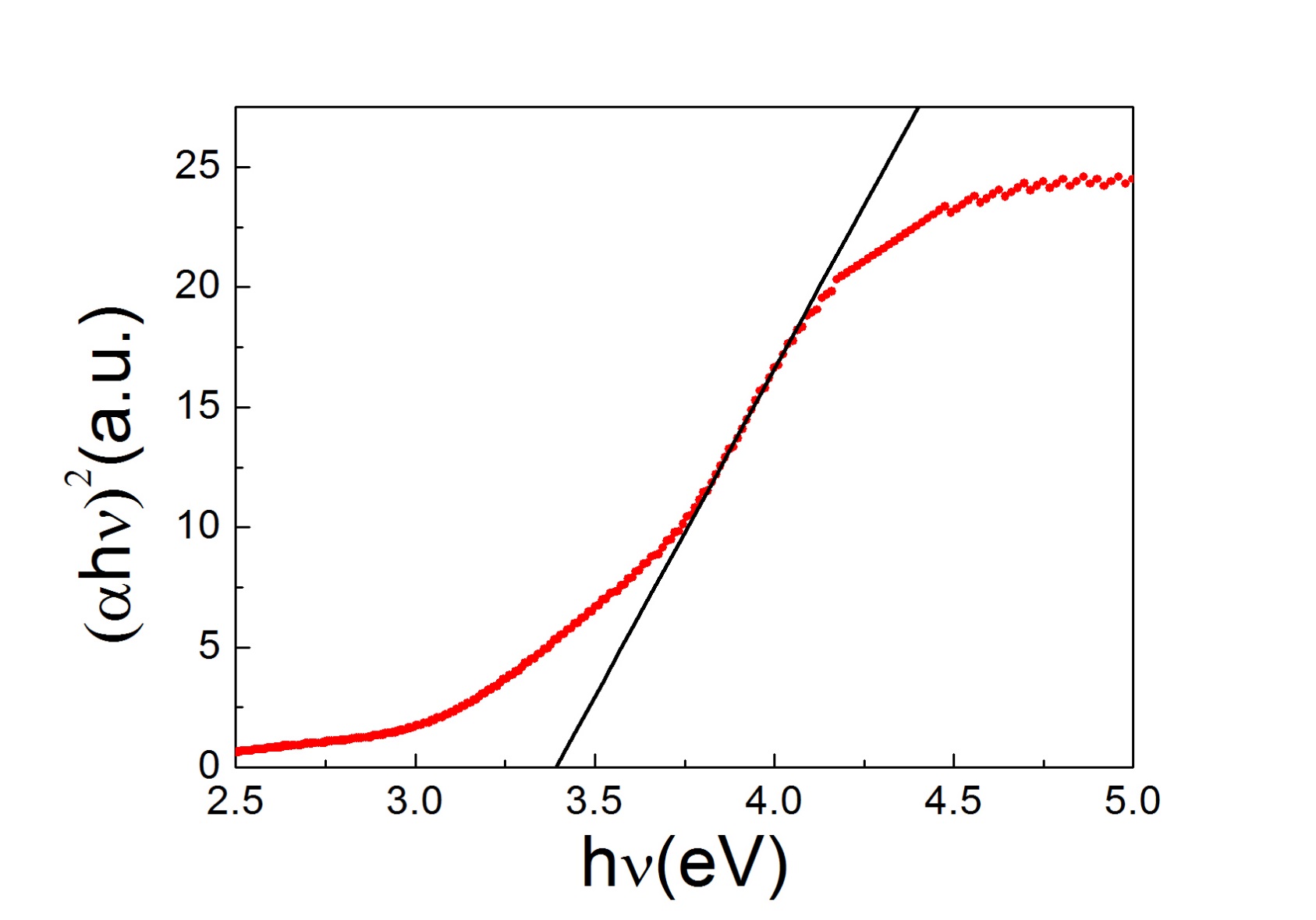


Fig. S3. UV-visible absorption spectra of the as-synthesized Ba3(Nb5.4a0.6)Si4O26, and Tauc plot for calculating band gaps *Eg* by extrapolation of the linear portion of the plots of (*αhν*)2 vs. *hν*. Insert is the corresponding absorbance curve.

Fig. S4. UV-visible absorption spectra of the as-synthesized Ba3(Nb4.2Ta1.8)Si4O26, and Tauc plot for calculating band gaps *Eg* by extrapolation of the linear portion of the plots of (*αhν*)2 vs. *hν*. Insert is the corresponding absorbance curve.

Fig. S3. UV-visible absorption spectra of the as-synthesized Ba3(Nb5.4Ta0.6)Si4O26, and Tauc plot for calculating band gaps *Eg* by extrapolation of the linear portion of the plots of (*αhν*)2 vs. *hν*. Insert is the corresponding absorbance curve.

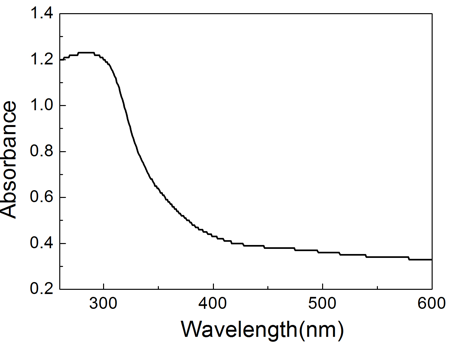
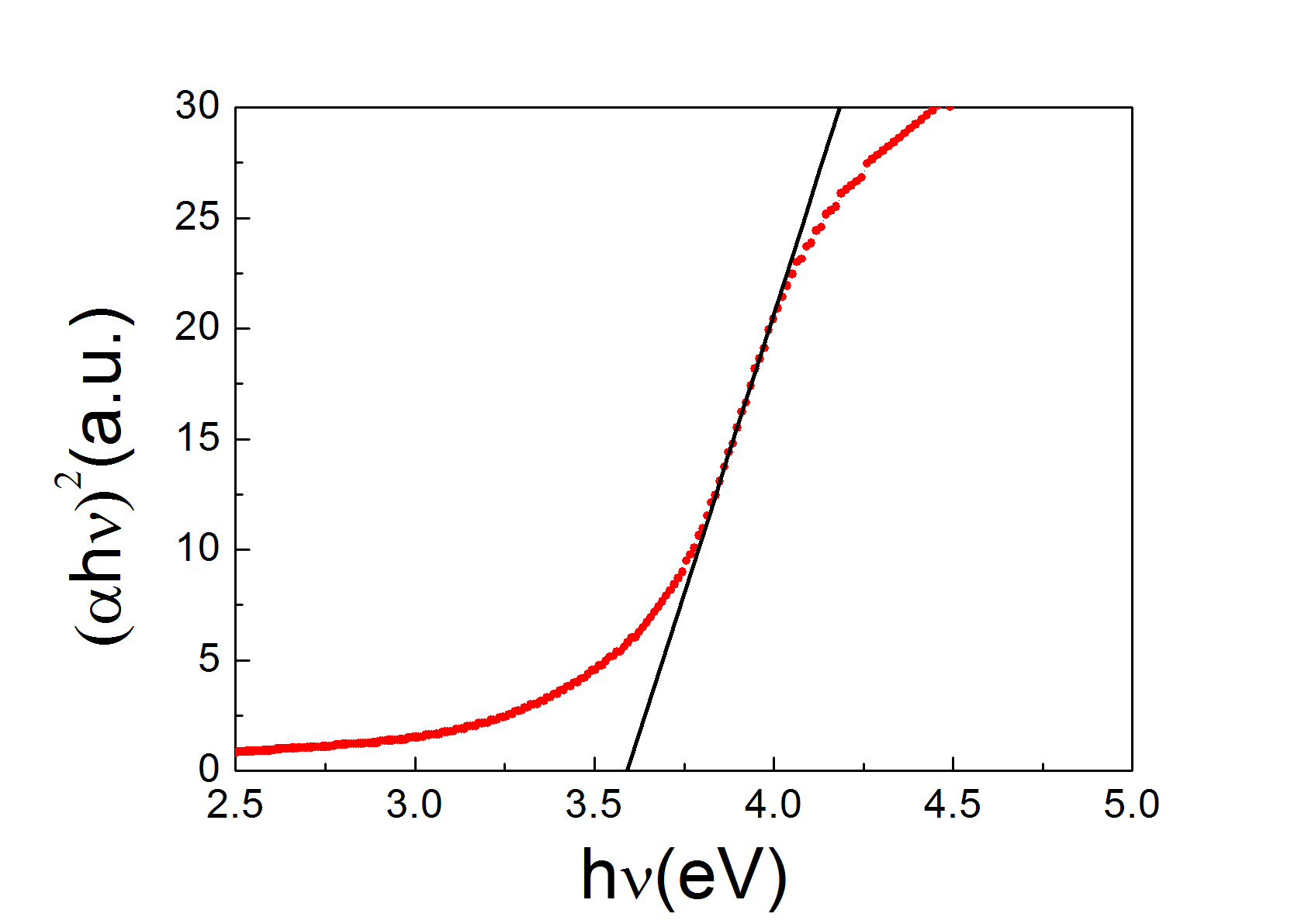


Fig. S4. UV-visible absorption spectra of the as-synthesized Ba3(Nb0.6Ta5.4) Si4O26, and Tauc plot

Fig. S4. UV-visible absorption spectra of the as-synthesized Ba3(Nb4.2Ta1.8)Si4O26, and Tauc plot for calculating band gaps *Eg* by extrapolation of the linear portion of the plots of (*αhν*)2 vs. *hν*.Insert is the corresponding absorbance curve.

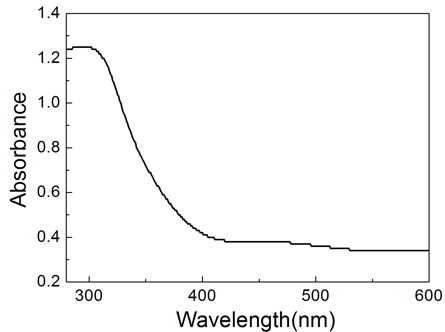
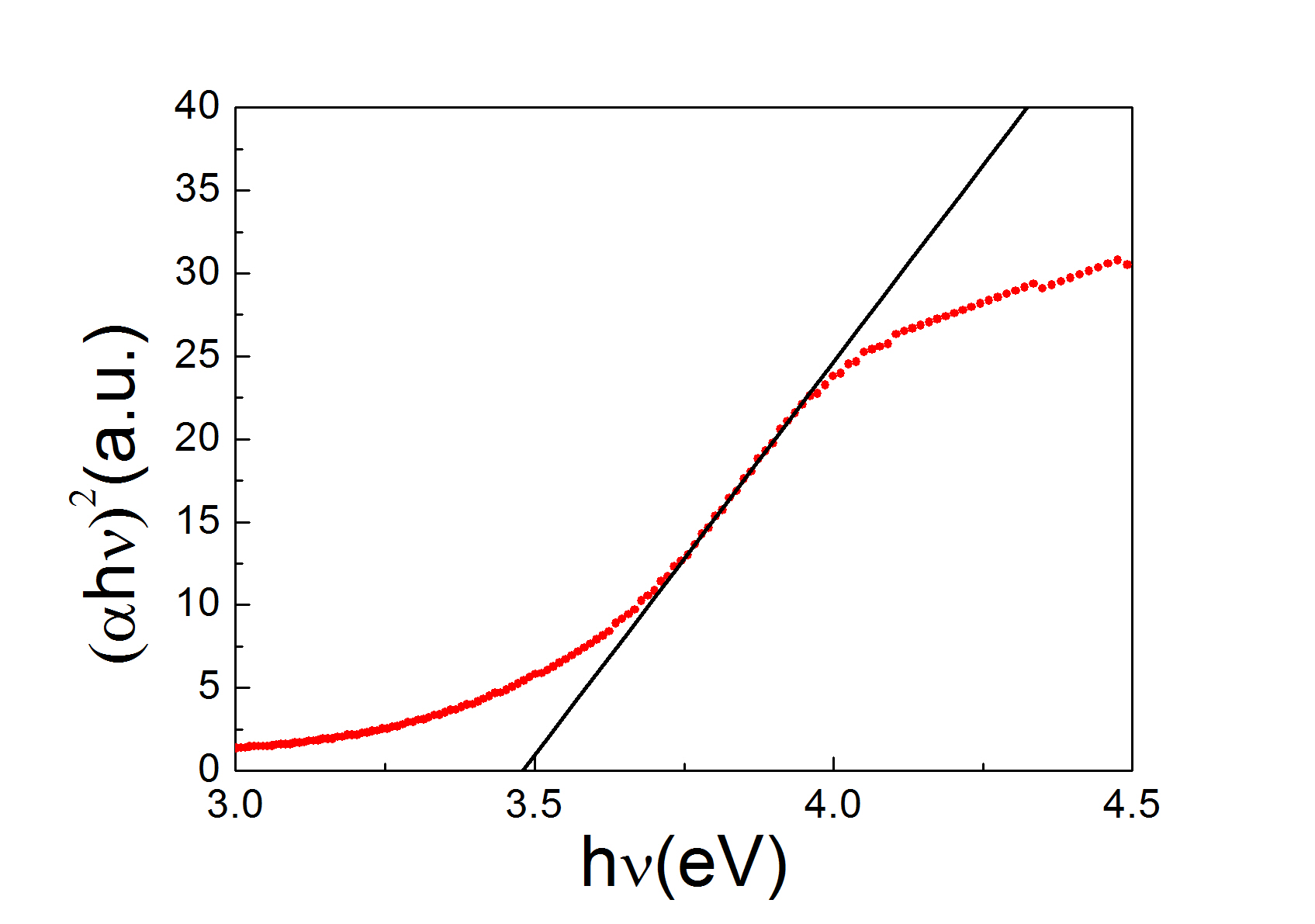


Fig. S5. UV-visible absorption spectra of the as-synthesized Ba3(Nb1.8Ta4.2)Si4O26, and Tauc plot for calculating band gaps *Eg* by extrapolation of the linear portion of the plots of (*αhν*)2 vs. *hν*.Insert is the corresponding absorbance curve.

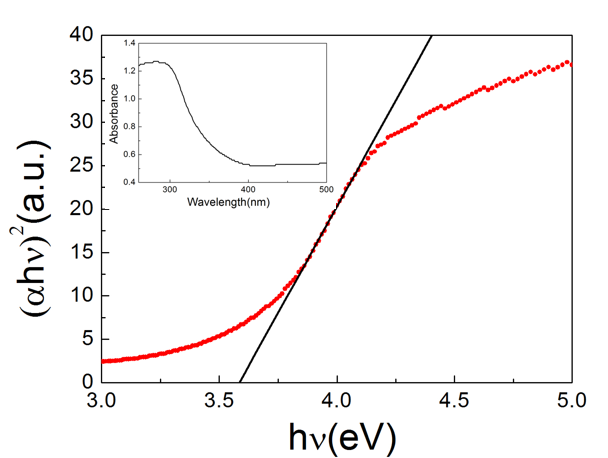


Fig. S6. UV-visible absorption spectra of the as-synthesized Ba3(Nb0.6Ta5.4) Si4O26, and Tauc plot for calculating band gaps *Eg* by extrapolation of the linear portion of the plots of (*αhν*)2 vs. *hν*.Insert is the corresponding absorbance curve.

Table S1. Atomic coordinates and displacement factors for compounds for Ba3(Nb6-xTax)Si4O26 *P-62m* (No. 189), *Z*=1. \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

Atom *x y z* Site Occ. Uiso Wyckoff

symbol

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(1) Ba3(Nb5.4Ta0.6)Si4O26

Ba1 0.6006(2) 0.0 0.5 1.0 0.0169(5) 3

Nb2/Ta3 0.2389(2) 0.0 0.243(2) 0.9/0.1 0.0268(5) 6

Si4 0.333 33 0.66667 0.2047(4) 1.0 0.022(3) 4

O5 0.333 33 0.66667 0.0 1.0 0.003(2) 2

O6 0.2775(13) 0.0 0.0 1.0 0.003(2) 3

O7 0.1918(7) 0.1918(7) 0.2309(10) 1.0 0.003(2) 6

O8 0.4897(4) 0.1758(6) 0.2753(6) 1.0 0.003(2) 12

O9 0.2162(13) 0.0 0.5 1.0 0.003(2) 3

(2) Ba3(Nb4.2Ta1.8)Si4O26

Ba1 0.6006(2) 0.0 0.5 1.0 0.0131(4) 3

Nb2 0.239 45(15) 0.0 0.2433 2) 0.7/0.3 0.0187(3) 6

Si4 0.333 33 0.666 67 0.2047(4) 1.0 0.020(2) 4

O5 0.333 33 0.666 67 0.0 1.0 0.0051 2

O6 0.2760(11) 0.0 0.0 1.0 0.0051 3

O7 0.1924(6) 0.1924(6) 0.2280(10) 1.0 0.0051 6

O8 0.4907(3) 0.1737(5) 0.2754(6) 1.0 0.0051 12

O9 0.2166(11) 0.0 0.5 1.0 0.0051 3

(3) Ba3(Nb3Ta3)Si4O2

Ba1 0.6008(3) 0.0 0.5 1.0 0.0127(5) 3

Nb2 0.2395(2) 0.0 0.2428(3) 0.5/0.5 0.0176(3) 6

Si4 0.333 33 0.666 67 0.2056(4) 1.0 0.026 (3) 4

O5 0.333 33 0.666 67 0.0 1.0 0.005 2

O6 0.2787(14) 0.0 0.0 1.0 0.005 3

O7 0.1934(7) 0.1934(7) 0.2250(12) 1.0 0.005 6

O8 0.4901(4) 0.1750(6) 0.2770(7) 1.0 0.005 12

O9 0.2140(14) 0.0 0.5 1.0 0.005 3

(4) Ba3(Nb1.8Ta4.2)Si4O26

Ba1 0.6011(3) 0.0 0.5 1.0 0.0159(6) 3

Nb2 0.2399(2) 0.0 0.2432(2) 0.3/0.7 0.0190(3) 6

Si4 0.33333 0.66667 0.2062(4) 1.0 0.027(4) 4

O5 0.33333 0.66667 0.0 1.0 0.003(2) 2

O6 0.2791(14) 0.0 0.0 1.0 0.003(2) 3

O7 0.1951(6) 0.1951(6) 0.2256(11) 1.0 0.003(2) 6

O8 0.4911(3) 0.1738(6) 0.2765(7) 1.0 0.003(2) 12 O9 0.2143(12) 0.0 0.5 1.0 0.003(2) 3

(5) Ba3(Nb0.6Ta5.4) Si4O26

Ba1 0.6016(3) 0.0 0.5 1.0 0.0194(6) 3

Nb2 0.239 81(12) 0.0 0.2447(2) 0.1/0.9 0.0190(3) 6

Si4 0.333 33 0.666 67 0.2076(4) 1.0 0.021(3) 4

O5 0.333 33 0.666 67 0.0 1.0 0.017(2) 2

O6 0.2837(13) 0.0 0.0 1.0 0.017(2) 3

O7 0.1947(6) 0.1947(6) 0.2251(10) 1.0 0.017(2) 6

O8 0.4906(3) 0.1761(6) 0.2804(6) 1.0 0.017(2) 12

O9 0.2116(11) 0.0 0.5 1.0 0.017(2) 3

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Table S2. Bond angles for Ba3(Nb6-xTax)Si4O26, *P-62m* (No. 189), *Z*=1, M=(Ta/Nb)

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

Bond angles (° )

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(1) x=0.6 (2)x=1.8 (3)x=3.0 (4)x=4.2 (5)x=5.4

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O5-Si4-O8 x3 110.1(2) 110.0(2) 110.2(2) 109.9(2) 110.5(2)

O8-Si4-O8 x3 108.8(2) 108.9(2) 108.8(2) 109.1(2) 108.4(2)

O6-M3-O7 x2 93.9(3) 92.9(3) 92.9(4) 92.9(3) 93.2(3)

O6-M3-O8 x2 89.5(2) 89.9(2) 89.8(2) 89.5(2) 89.2(2)

O7-M3-O7 98.4(4) 98.4(3) 98.8(4) 99.5(3) 99.2(3)

O7-M3-O9 x2 89.0(2) 89.7(2) 89.8(3) 89.7(2) 89.6(2)

O7-M3-O8 x2 88.0(2) 88.7(2) 88.1(2) 88.2(2) 87.7(3)

O8-M3-O8 85.3(4) 84.1(3) 84.8(4) 84.1(4) 85.3(4)

O8-M3-O9 x2 87.1(3) 87.2(2) 87.2(3) 87.5(3) 87.5(2)

Si-O5-Si 180 180 180 180 180

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