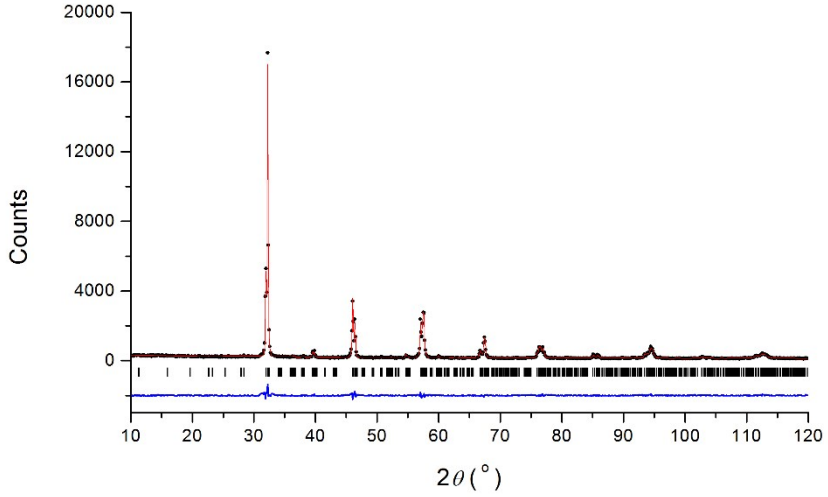
Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.


# Supplementary Information

(a)




(b)

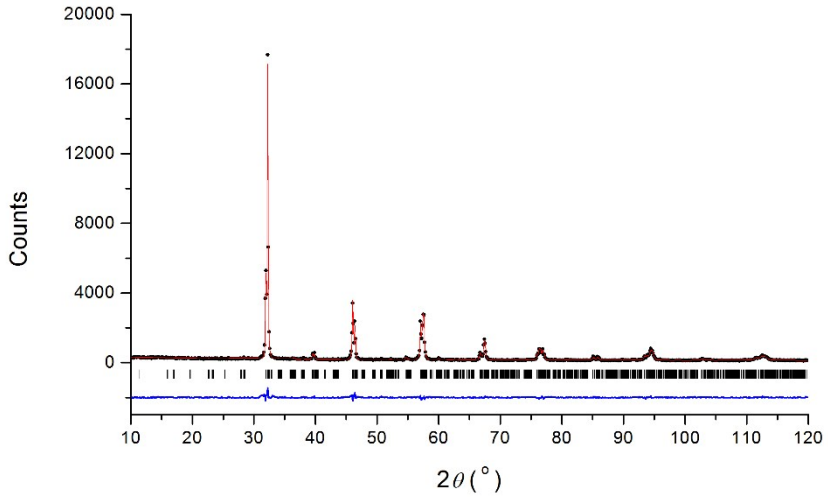



Fig. S1. Fitted X-ray powder diffraction profiles for $AgNbO_3$ (a) *Pbcm* and (b) $Pb2_1m$ models, showing observed (points), fitted (line) and difference (lower) profiles. Reflection positions are indicated by markers.

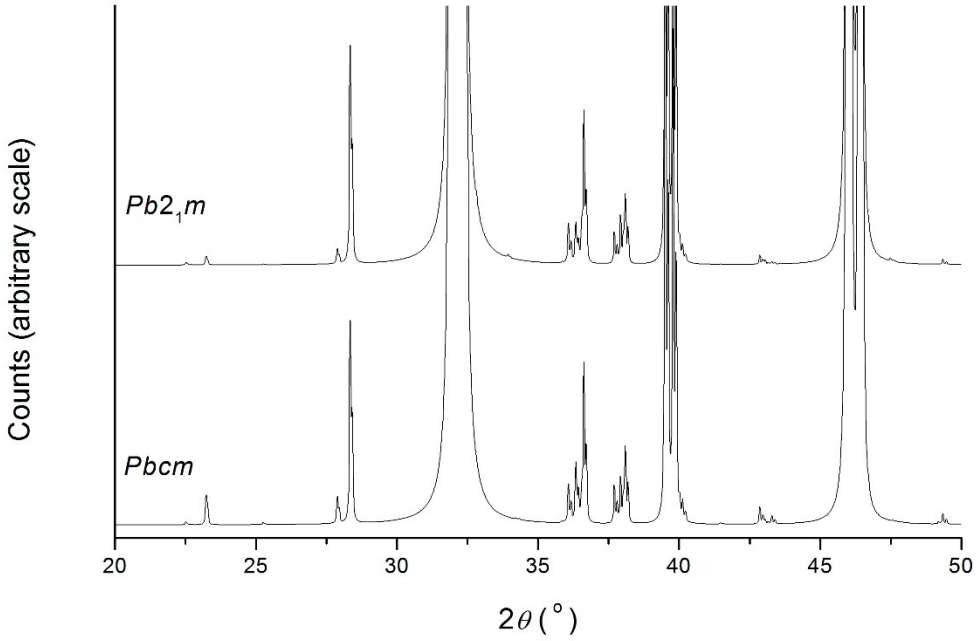



Fig. S2. Comparison of calculated X-ray diffraction patterns based on the published data for polar (ref.19) and non-polar (ref.17) structure models for $AgNbO_3$.

**Table S1**. Refined structural parameters for $AgNbO_3$ ground ceramic powder for (a) *Pbcm* and (b) $Pb2_1m$ models. Estimated Standard deviations are given in parentheses.

(a)

| Atom | Site | *x* | *y* | *z* | Occ. | $U_{iso}$ (Å$^2$) |
|---|---|---|---|---|---|---|
| Ag(1) | 4*d* | 0.7534(24) | 0.2309(10) | 0.75 | 1 | 0.0249(7) |
| Ag(2) | 4*c* | 0.7540(24) | 0.25 | 0.5 | 1 | 0.0249(7) |
| Nb | 8*e* | 0.7484(20) | 0.7290(8) | 0.6254(5) | 1 | 0.0206(8) |
| O(1) | 4*d* | 0.719(15) | 0.770(5) | 0.75 | 1 | 0.034(3) |
| O(2) | 4*c* | 0.796(13) | 0.75 | 0.5 | 1 | 0.034(3) |
| O(3) | 8*e* | 0.454(5) | 0.547(8) | 0.612(2) | 1 | 0.034(3) |
| O(4) | 8*e* | 0.992(6) | 0.509(7) | 0.639(2) | 1 | 0.034(3) |

(b)

| Atom | Site | *x* | *y* | *z* | Occ. | $U_{iso}$ (Å$^2$) |
|---|---|---|---|---|---|---|
| Ag(1)* | 4*c* | 0.7468 | 0.2601 | 0.7499 | 1 | 0.0281(9) |
| Ag(2) | 2*b* | 0.7427(34) | 0.2491(25) | 0.5 | 1 | 0.0281(9) |
| Ag(3) | 2*a* | 0.7492(34) | 0.2866(24) | 0 | 1 | 0.0281(9) |
| Nb(1) | 4*c* | 0.7574(27) | 0.7347(22) | 0.6235(9) | 1 | 0.017(1) |
| Nb(2) | 4*c* | 0.2543(28) | 0.2770(33) | 0.1244(10) | 1 | 0.017(1) |
| O(1) | 4*c* | 0.694(12) | 0.753(12) | 0.731(2) | 1 | 0.025 |
| O(2) | 2*b* | 0.755(19) | 0.813(10) | 0.5 | 1 | 0.025 |
| O(3) | 4*c* | 0.464(16) | 0.578(11) | 0.652(4) | 1 | 0.025 |
| O(4) | 4*c* | 0.016(16) | 0.566(12) | 0.623(4) | 1 | 0.025 |
| O(5) | 2*a* | 0.161(21) | 0.304(12) | 0 | 1 | 0.025 |
| O(6) | 4*c* | 0.018(13) | 0.030(11) | 0.147(4) | 1 | 0.025 |
| O(7) | 4*c* | 0.490(17) | 0.534(13) | 0.110(4) | 1 | 0.025 |

*Parameters fixed to define origin.