## -SUPLEMENTARY INFORMATION-

# Experimental corroboration of the thermoelectric performance of $Bi_2PdO_4$ oxide and Pb- doped derivatives

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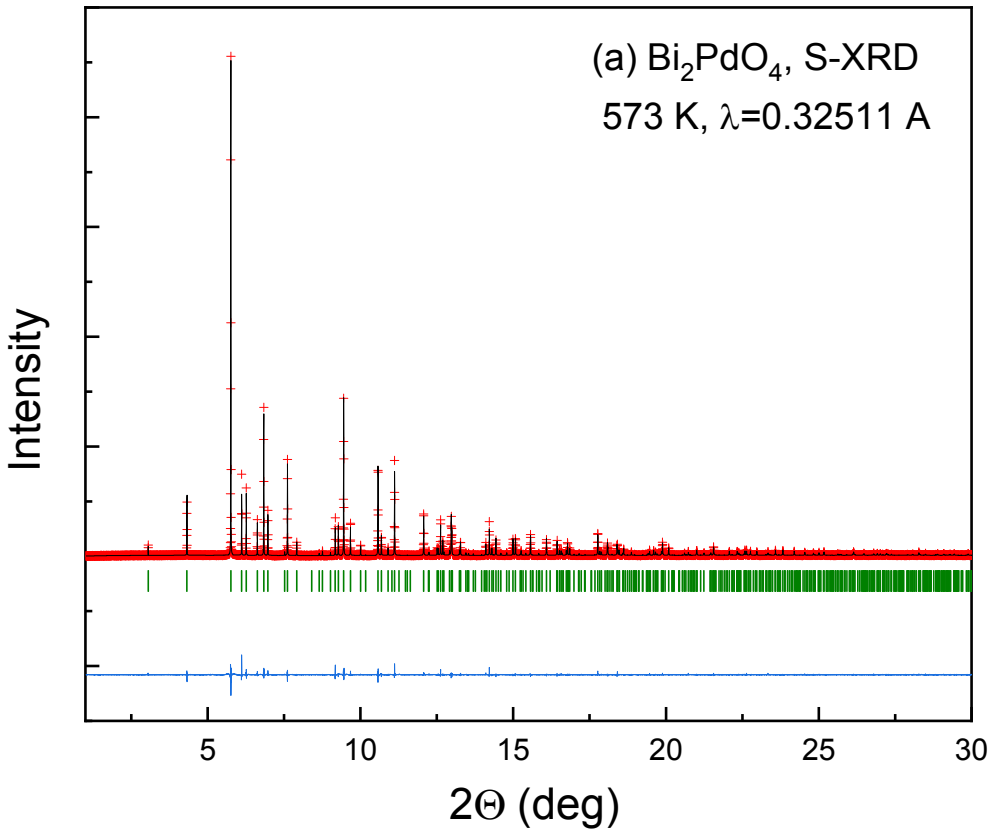
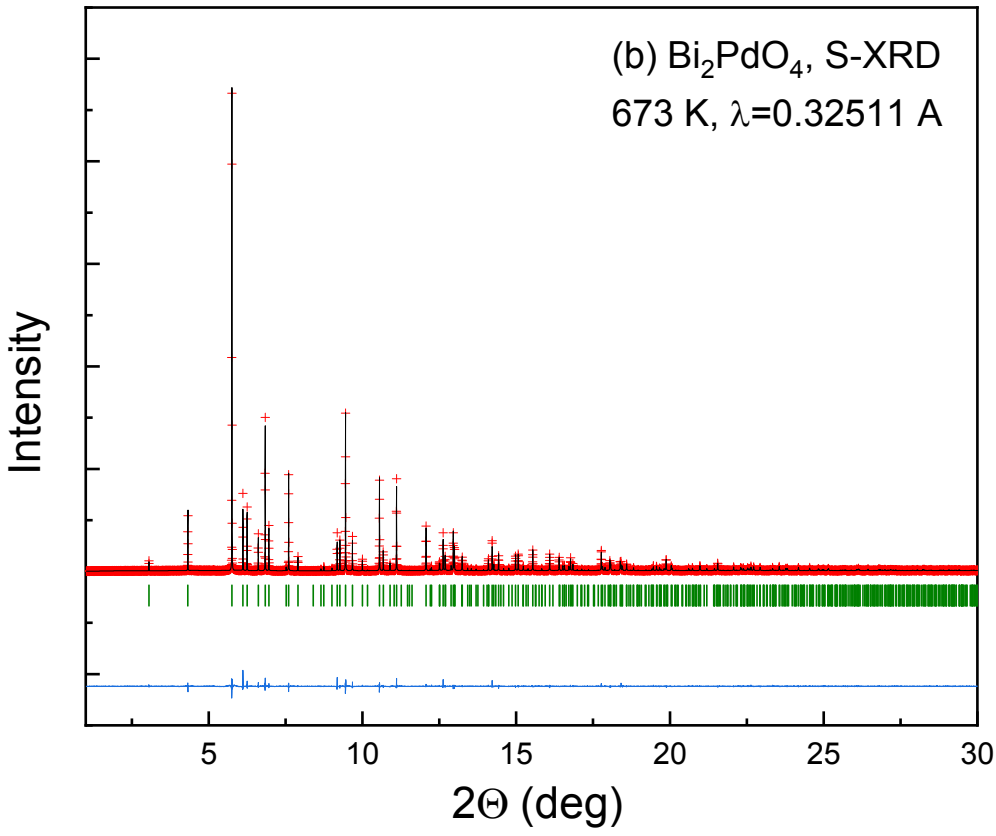
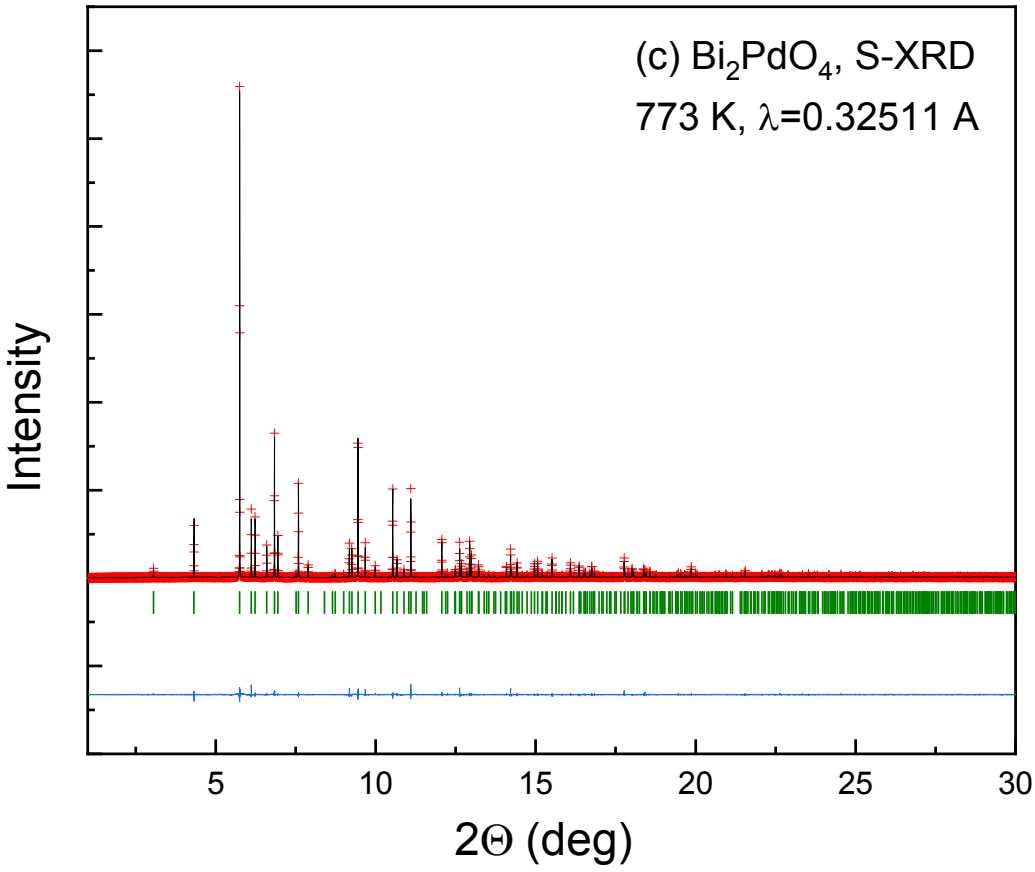
**Table S1.** Unit-cell, atomic positions, thermal parameters and reliability factors for $Bi_{1.9}Pb_{0.1}PdO_4$ obtained from SXRD data at room temperature, 573, 673 and 773 K.

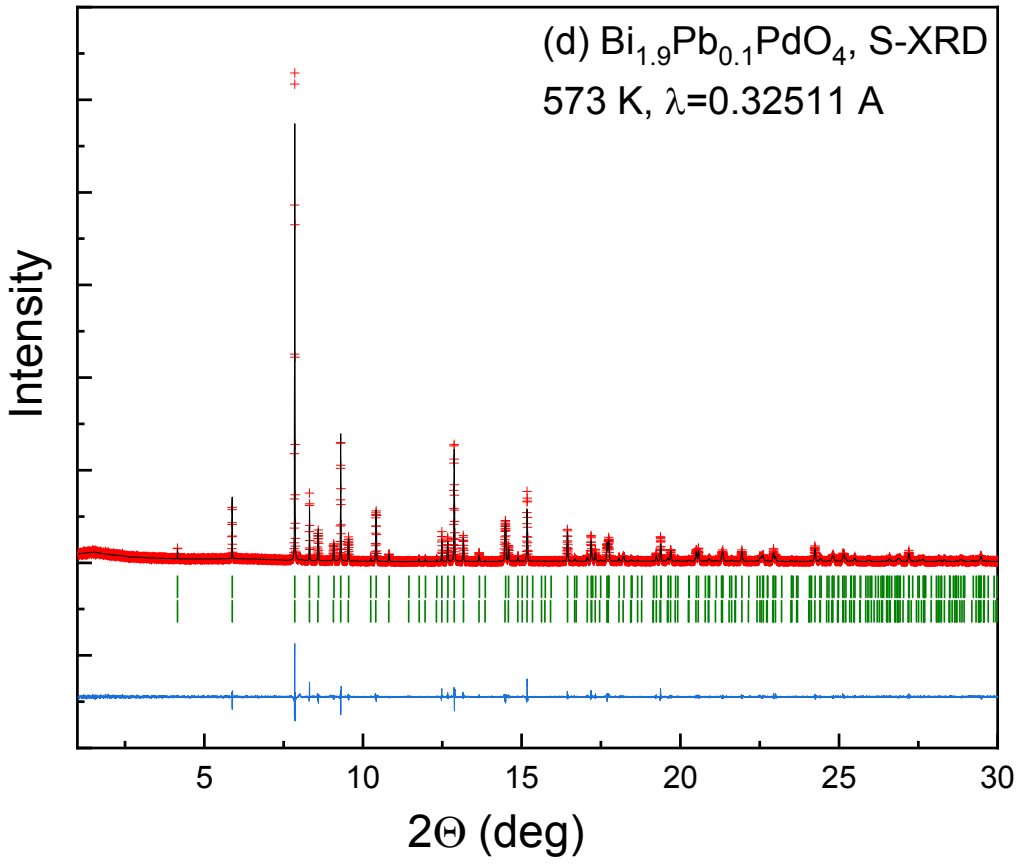
| | **298 K** | **573 K** | **673 K** | **773 K** |
|---|---|---|---|---|
| a (Å) | 8.62457(6) | 8.62397(5) | 8.62346(5) | 8.62279(4) |
| c (Å) | 5.90929(5) | 5.94980(4) | 5.96554(4) | 5.98211(4) |
| V (Å$^3$) | 439.551(5) | 442.504(5) | 443.622(5) | 444.785(4) |
| **Bi** 8f (x,-x, ¼) | | | | |
| x | -0.0799(1) | -0.0793(1) | -0.0792(1) | -0.0788 (1) |
| Biso | 1.05(4) | 1.59(4) | 1.78(4) | 2.12(4) |
| **Pd/Ag** 4c (¼,¼,z) | | | | |
| z | 0.0832(7) | 0.0829(7) | 0.0824(7) | 0.0832(7) |
| Biso | 0.5 (1) | 0.97(9) | 1.1 (1) | 1.3 (1) |
| **O** 16g (x,y,z) | | | | |
| x | 0.472(3) | 0.472(2) | 0.464(2) | 0.465(2) |
| y | 0.133(2) | 0.136(2) | 0.137(2) | 0.139(2) |
| z | 0.089(4) | 0.094(3) | 0.092(3) | 0.089(3) |
| Biso | 2.7(6) | 2.3(6) | 1.7(5) | 1.7(5) |
| **Reliability factors** | | | | |
| $R_{Bragg}$(%) | 11.7 | 17.1 | 17.9 | 18.5 |
| $R_p$(%) | 14.9 | 13.5 | 13.9 | 15.5 |
| $R_{wp}$(%) | 18.7 | 16.9 | 17.3 | 19.4 |
| Rexp(%) | 14.3 | 14.1 | 14.01 | 13.87 |
| $\chi^2$ | 1.76 | 1.44 | 1.52 | 1.95 |

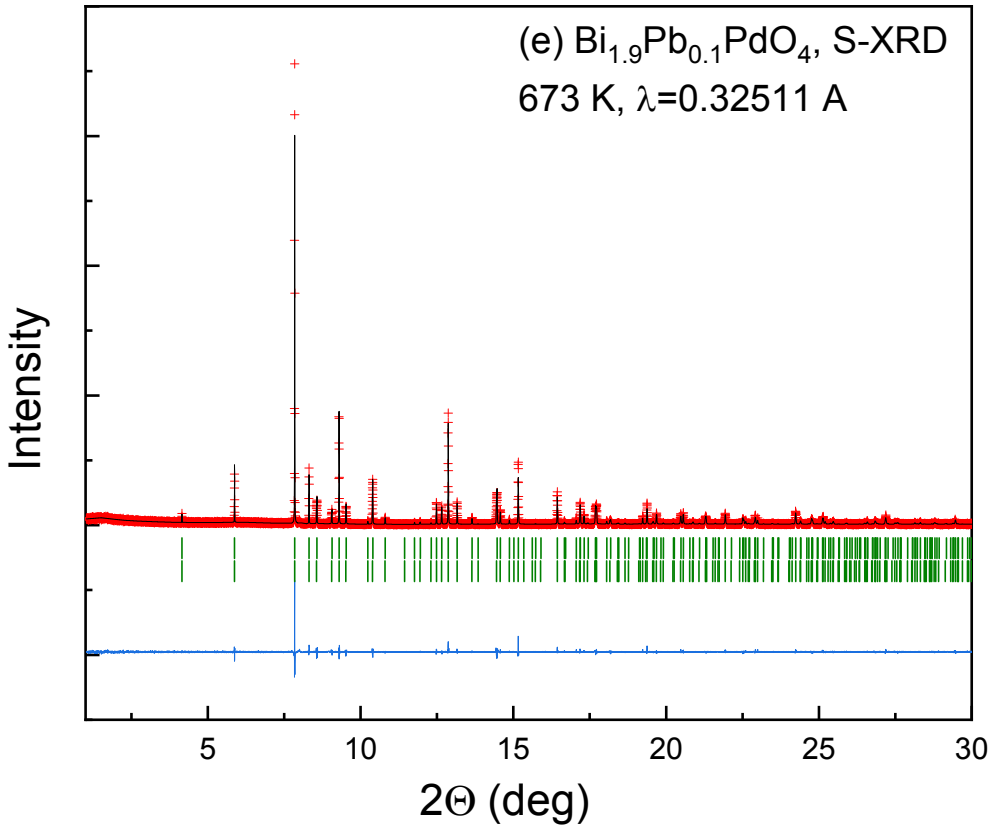
**Figure S1.** Observed (crosses), calculated (solid line) and difference (bottom) S-XRD Rietveld profiles for $Bi_2PdO_4$ at (a) 573, (b) 673 and (c) 773 K and $Bi_{1.90}Pb_{0.1}PdO_4$ at (d) 573, (e) 673 and (f) 773 K collected at MSPD diffractometer (ALBA). The vertical green markers represent the positions of the space-group-allowed Bragg reflections

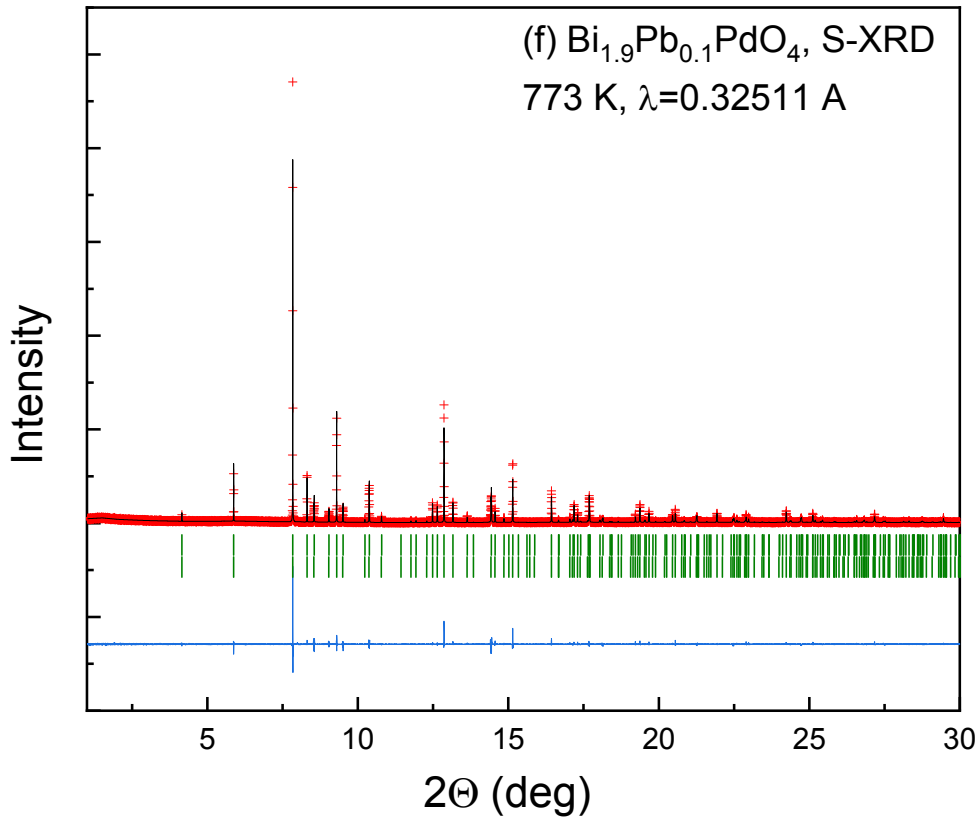



(c) Bi2PdO4, S-XRD
773 K, λ=0.32511 A
Intensity
5
10
15
20
25
30
2Θ (deg)


(d) Bi1.9Pb0.1PdO4, S-XRD
573 K, λ=0.32511 A
Intensity
5
10
15
20
25
30
2Θ (deg)


(e) $Bi_{1.9}Pb_{0.1}PdO_4$, S-XRD
673 K, λ=0.32511 A
Intensity
5
10
15
20
25
30
2Θ (deg)


(f) $Bi_{1.9}Pb_{0.1}PdO_4$, S-XRD
773 K, λ=0.32511 A
Intensity
5
10
15
20
25
30
2Θ (deg)