Structure and electrical properties of layered perovskite type $Pr_2Ti_2O_7$: Experimental and theoretical investigations

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Supplementary Information

SI-I: Rietveld refinement plots of powder XRD data in different structural models.

SI-II: Calculated structural parameters of different model structures PTO. Parameters obtained by Rietveld refinements are included in each Table.

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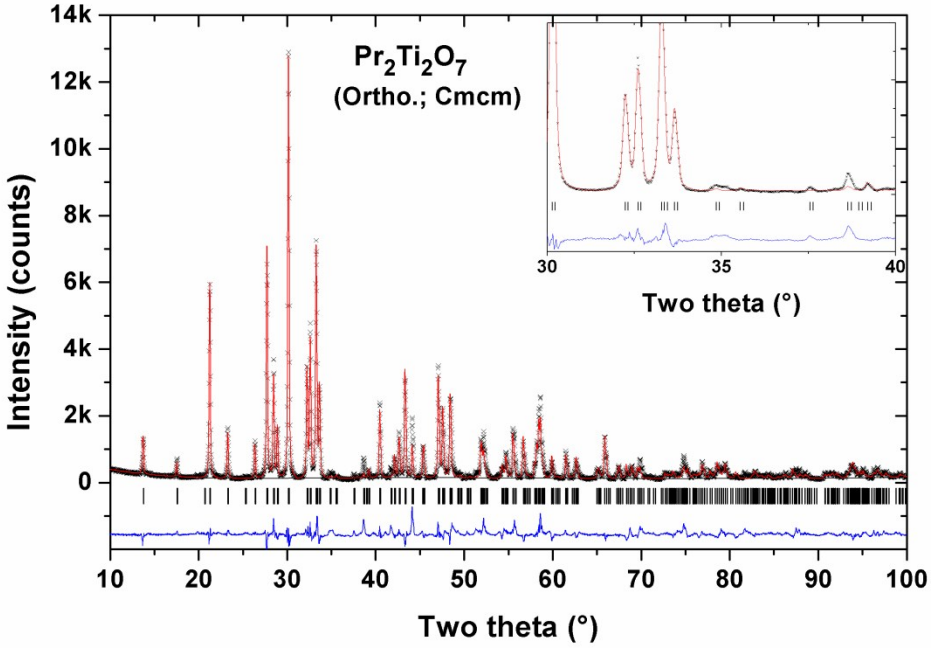
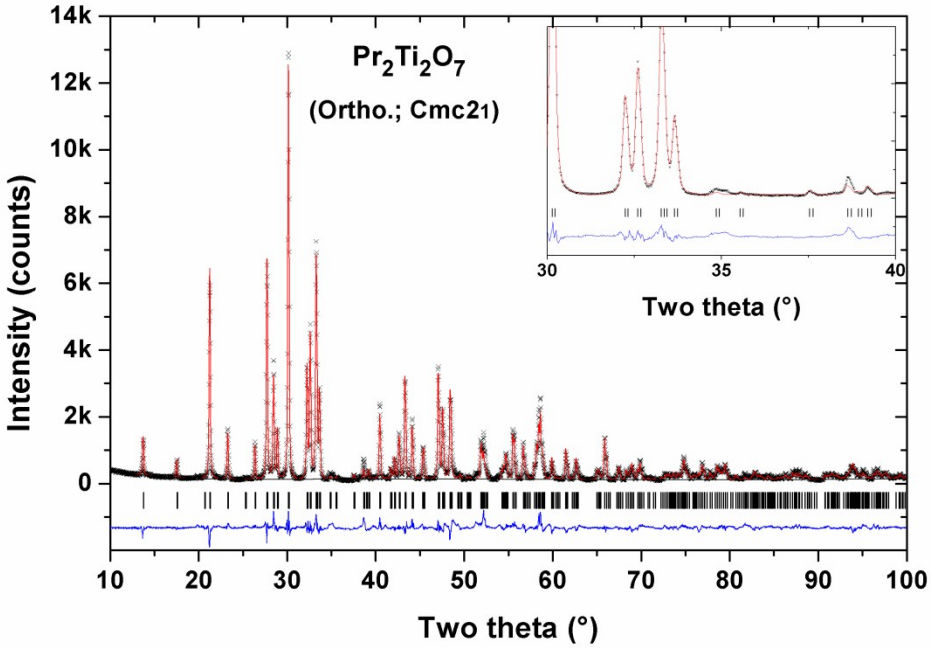
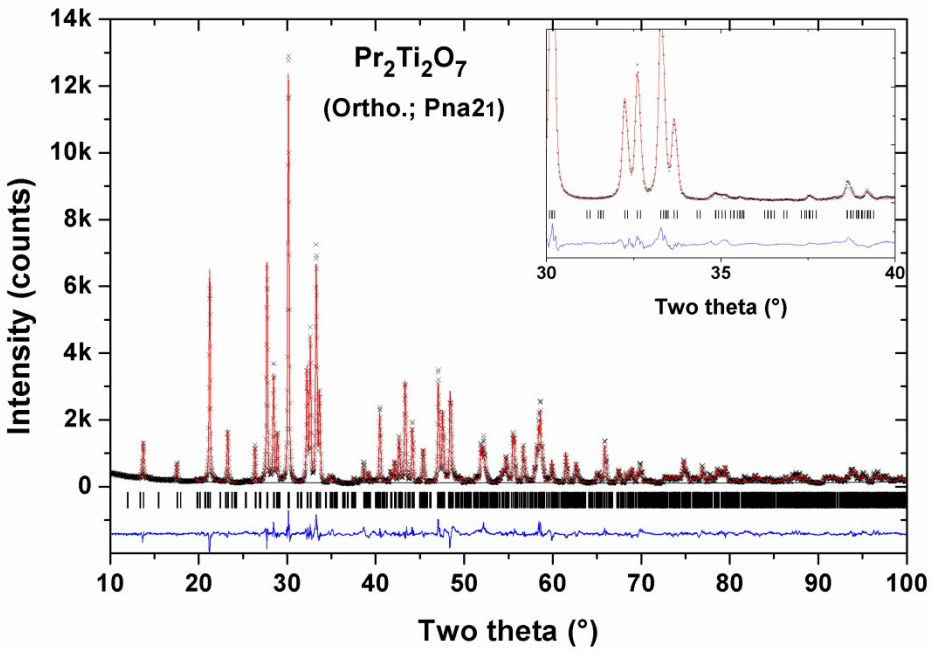
SI-I: Rietveld refinement plots of powder XRD data in different structural models.



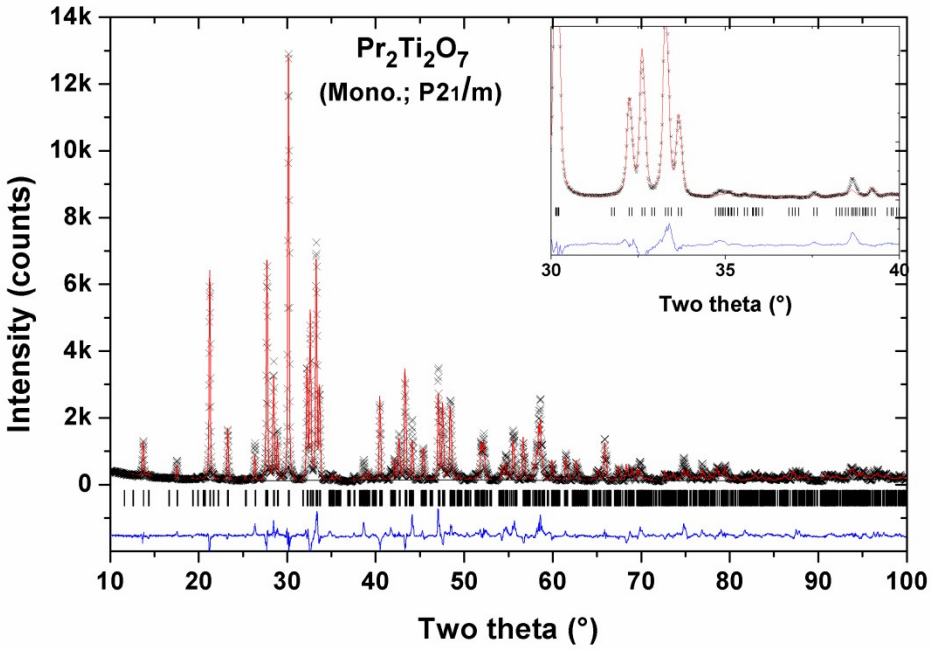
(a). Orthorhombic, Cmcm



(b). Orthorhombic, $Cmc2_1$



(c). Orthorhombic, $Pna2_1$



(d). Monoclinic, $P2_1/m$

SI-II. Calculated structural parameters of different model structures PTO. Parameters obtained by Rietveld refinements are included in each Table.

(a). Orthorhombic (Cmcm)

Atoms	Wyc	x	y	z	Uiso	Occ.
Pr1	4	0 0	0.44646(8) 0.44863	0.75 0.75	0.0348(8)	1
Pr2	4	0 0	0.29895(10) 0.28652	0.25 0.25	0.0471(10)	1
Ti1	4	0.5 0	0.44075(20) 0.44277	0.25 0.25	0.01052	1
Ti2	4	0.5 0	0.33760(20) 0.34131	0.75 0.75	0.01025	1
O1	4	0.5 0.5	0.5 0.5	0.5 0.5	0.1011(35)	1
O2	4	0 0	0.4532(9) 0.45686	0.25 0.25	0.1011(35)	1
O3	4	0 0	0.3476(8) 0.35237	0.75 0.75	0.1011(35)	1
O4	8	0.5 0.5	0.3986(4) 0.30014	0.9831(21) 0.98939	0.1011(35)	1
O5	8	0.5 0.5	0.2907(5) 0.28914	0.9797(22) 0.98858	0.1011(35)	1

Space Group: Cmcm
a = 3.8834(2), b = 25.8274(15), c = 5.5236(3), V = 554.01(5)
a = 3.86719, b = 26.51346, c = 5.62100

(b). Orthorhombic ($Cmc2_1$)

Atoms	Wyc	x	y	z	Uiso	Occ.
Pr1	4	0 0	0.44627(7) 0.4536	0.7536(13) 0.7107	0.0261(6)	1
Pr2	4	0 0	0.29813(9) 0.2981	0.1888(14) 0.1438	0.0428(9)	1
Ti1	4	0.5 0.5	0.43839(18) 0.4324	0.2487(18) 0.2385	0.0119(16)	1
Ti2	4	0.5 0.5	0.33754(18) 0.3364	0.7185(16) 0.6950	0.0139(17)	1
O1	4	0.5 0.5	0.5114(7) 0.5186	0.469(4) 0.4888	0.0448(25)	1
O2	4	0.5 0.5	0.4112(5) 0.4091	0.5615(24) 0.5626	0.0448(25)	1
O3	4	0.5 0.5	0.2894(8) 0.2985	0.493(4) 0.4350	0.0448(25)	1
O4	4	0 0	0.4518(6) 0.4508	0.226(7) 0.2910	0.0448(25)	1
O5	4	0 0	0.3446(6) 0.3511	0.651(4) 0.7618	0.0448(25)	1
O6	4	0.5 0.5	0.3858(7) 0.3719	0.0483(26) 0.0925	0.0448(25)	1
O7	4	0.5 0.5	0.2874(9) 0.2784	0.955(4) 0.8948	0.0448(25)	1

a = 3.85753(7), b = 25.7195(5), c = 5.48771(12), V = 544.456

a = 3.78373, b = 25.81822, c = 5.87300

(c). Orthorhombic ($Pna2_1$)

Atoms	Wyc.				
Ti1	4	0.09082(26) 0.0900	0.1311(11) 0.1173	0.791(5) 0.7924	0.02798
Ti2	4	0.18646(27) 0.1900	0.1174(12) 0.1720	0.2643(11) 0.2653	0.02798
Ti3	4	0.31069(25) 0.3109	0.1219(12) 0.1232	0.7519(11) 0.7632	0.02798
Ti4	4	0.41469(26) 0.4126	0.1250(12) 0.1288	0.2800(12) 0.2998	0.02798
La1	4	0.05189(13) 0.5594	0.3756(16) 0.3805	0.2926(8) 0.2913	0.0411(11)
La2	4	0.19681(12) 0.2056	0.3777(12) 0.3749	0.7540(9) 0.7605	0.0186(7)
La3	4	0.30401(13) 0.3109	0.3773(13) 0.3767	0.2480(9) 0.2489	0.0296(9)
La4	4	0.45597(14) 0.4644	0.3781(14) 0.3722	0.8346(7) 0.8621	0.0351(10)
O1	4	0.0435(7) 0.0358	0.156(6) 0.1484	0.5465(14) 0.5755	0.0279(22)
O2	4	0.0370(6) 0.0471	0.093(5) 0.1018	-0.0452(16) 0.0601	0.0279(22)
O3	4	0.0945(10) 0.0970	0.3692(12) 0.3761	0.8782(17) 0.8561	0.0279(22)
O4	4	0.1286(6) 0.1359	0.228(27) 0.1854	0.4388(13) 0.4598	0.0279(22)
O5	4	0.1636(5) 0.1587	0.126(8) 0.1023	0.9388(14) 0.9463	0.0279(22)
O6	4	0.2100(8) 0.2040	0.3475(12) 0.3753	0.2568(18) 0.1727	0.0279(22)
O7	4	0.2366(5) 0.2397	0.154(5) 0.1644	0.5282(16) 0.5202	0.0279(22)
O8	4	0.2555(5) 0.2605	0.117(8) 0.0868	0.0200(16) 0.0201	0.0279(22)
O9	4	0.3072(10) 0.3048	0.3700(12) 0.3755	0.8560(17) 0.8162	0.0279(22)
O10	4	0.3463(5) 0.3405	0.140(7) 0.1488	0.4491(15) 0.4433	0.0279(22)
O11	4	0.3594(5) 0.3652	0.070(4) 0.0644	0.9633(15) 0.9565	0.0279(22)
O12	4	0.4120(10) 0.4028	0.3704(12) 0.3751	0.3438(18) 0.1997	0.0279(22)
O13	4	0.4490(8) 0.4439	0.133(9) 0.1548	0.5569(15) 0.5849	0.0279(22)
O14	4	0.4671(6) 0.4703	0.111(8) 0.1050	0.0402(16) 0.0924	0.0279(22)

a = 25.7197(4), b = 7.71509(12), c = 5.48767(9), V = 1088.919(29)

a = 26.31000, b = 7.75500, c = 5.56000

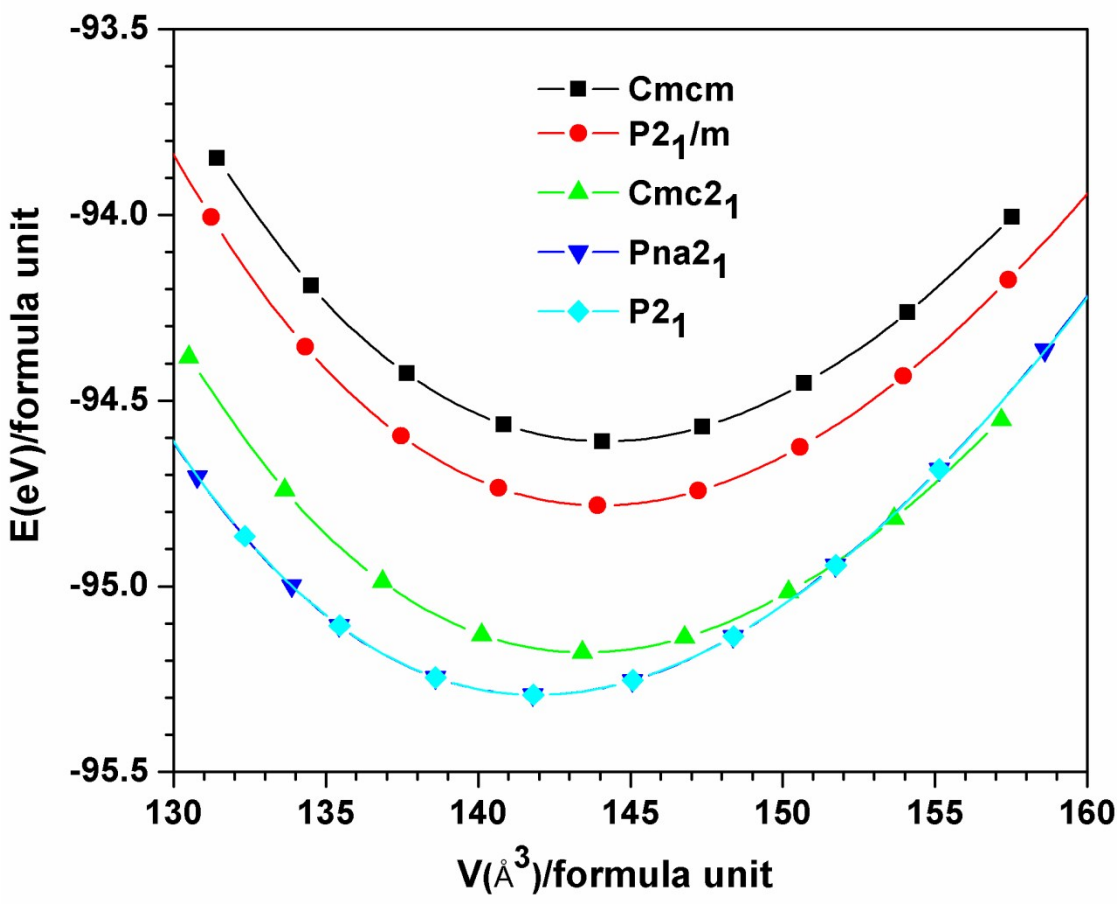
(d). Monoclinic ($P2_1/m$)

Atoms	Wyc	x	y	z	Uiso	Occ.
Pr1	2	0.7324(14) 0.7269	0.25 0.25	0.88633(35) 0.8909	0.0381(15)	1
Pr1a	2	0.2323(12) 0.2269	0.25 0.25	0.89985(33) 0.8909	0.0235(12)	1
Pr2	2	0.8448(15) 0.8555	0.25 0.25	0.4143(4) 0.4270	0.0707(22)	1
Pr2a	2	0.3478(13) 0.3555	0.25 0.25	0.39153(33) 0.4270	0.0264(12)	1
Ti1	2	0.5258(17) 0.5264	0.25 0.25	0.1146(7) 0.1104	0.03523	1
Ti1a	2	0.0278(17) 0.0264 0	0.25 0.25	0.1151(7) 0.1104	0.03523	1
Ti2	2	0.9242(17) 0.9313	0.25 0.25	0.6763(8) 0.6826	0.03523	1
Ti2a	2	0.4272(17) 0.4313	0.25 0.25	0.6802(8) 0.6826	0.03523	1
O3	2	0 0	0 0	0 0	0.0854(35)	1
O3a	2	0.5 0.5	0 0	0 0	0.0854(35)	1
O4	2	0.7796(18) 0.7731	0.25 0.25	0.1288(29) 0.0921	0.0854(35)	1
O4a	2	0.2661(19) 0.2731	0.25 0.25	0.0733(24) 0.0921	0.0854(35)	1
O5	2	0.6739(18) 0.6735	0.25 0.25	0.6758(29) 0.6952	0.0854(35)	1
O5a	2	0.1796(18) 0.1735	0.25 0.25	0.6929(29) 0.6952	0.0854(35)	1
O6	4	0.430(5) 0.4487	1.0308(23) 1.0159	0.8115(10) 0.7996	0.0854(35)	1
O6a	4	0.8906(33) 0.9487	0.9601(26) 0.9841	0.7790(11) 0.7996	0.0854(35)	1
O7	4	0.389(7) 0.3950	0.0378(32) 0.00676	0.5856(13) 0.5783	0.0854(35)	1
O7a	4	0.893(7) 0.8950	0.0185(30) 0.0068	0.5930(15) 0.5783	0.0854(35)	1

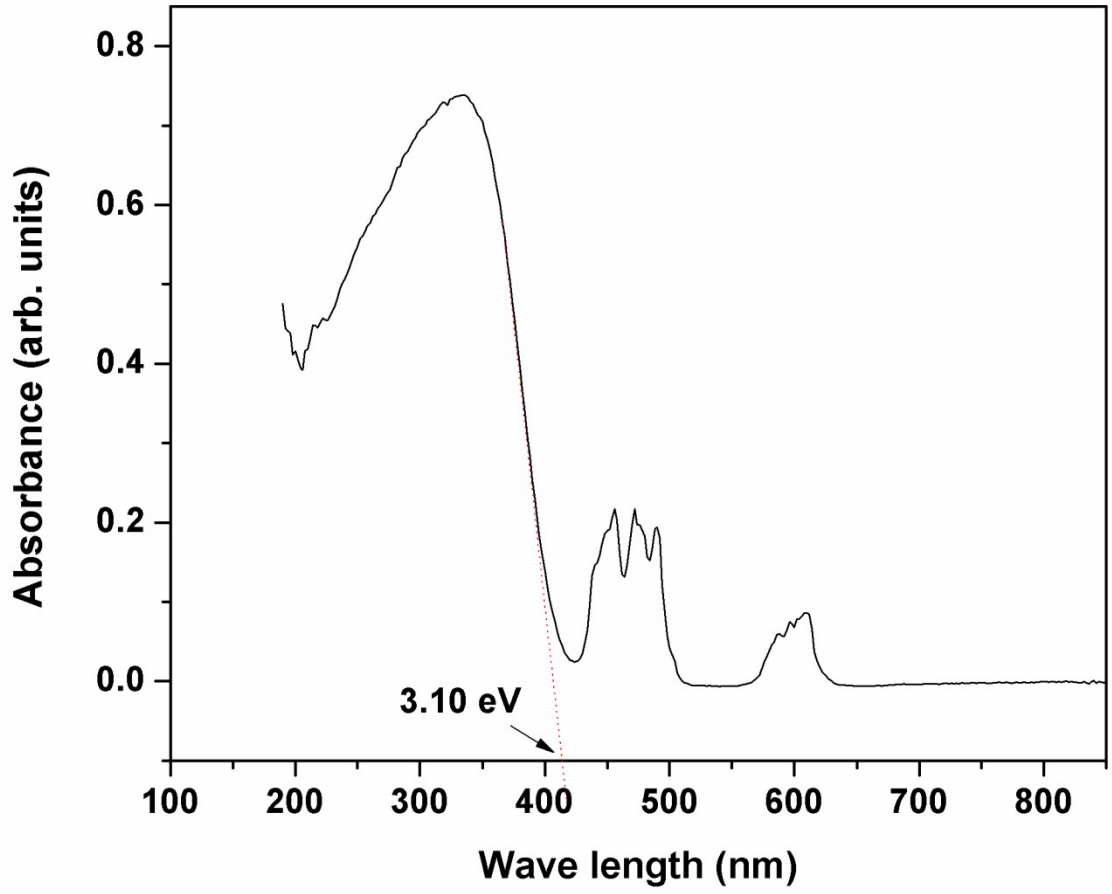
a = 7.71461(21), b = 5.48743(12), c = 13.0036(4), β = 98.531(7), V = 544.397(23)

a = 7.866463, b = 5.544969, c = 13.345535, β = 98.52855

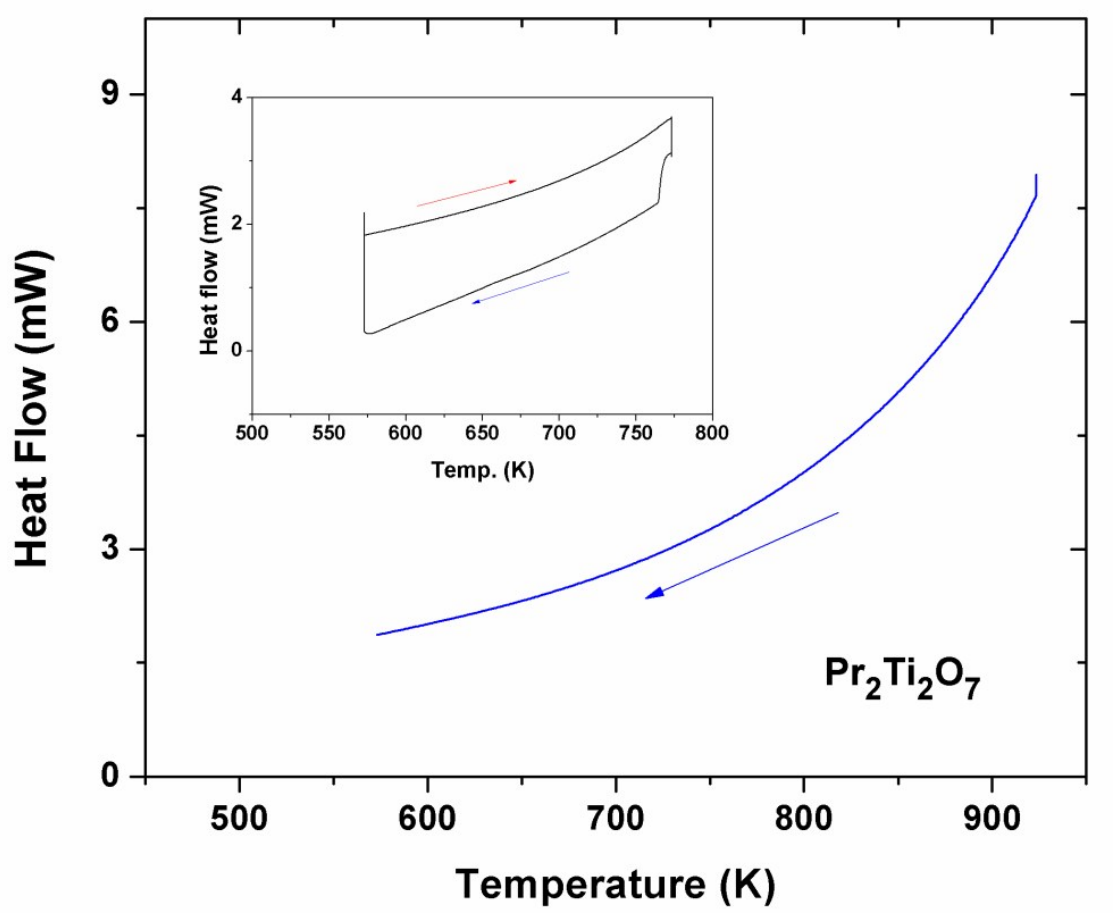
SI-III. Variation of energy (energy/formula unit) of PTO in different model structures with molar volume.



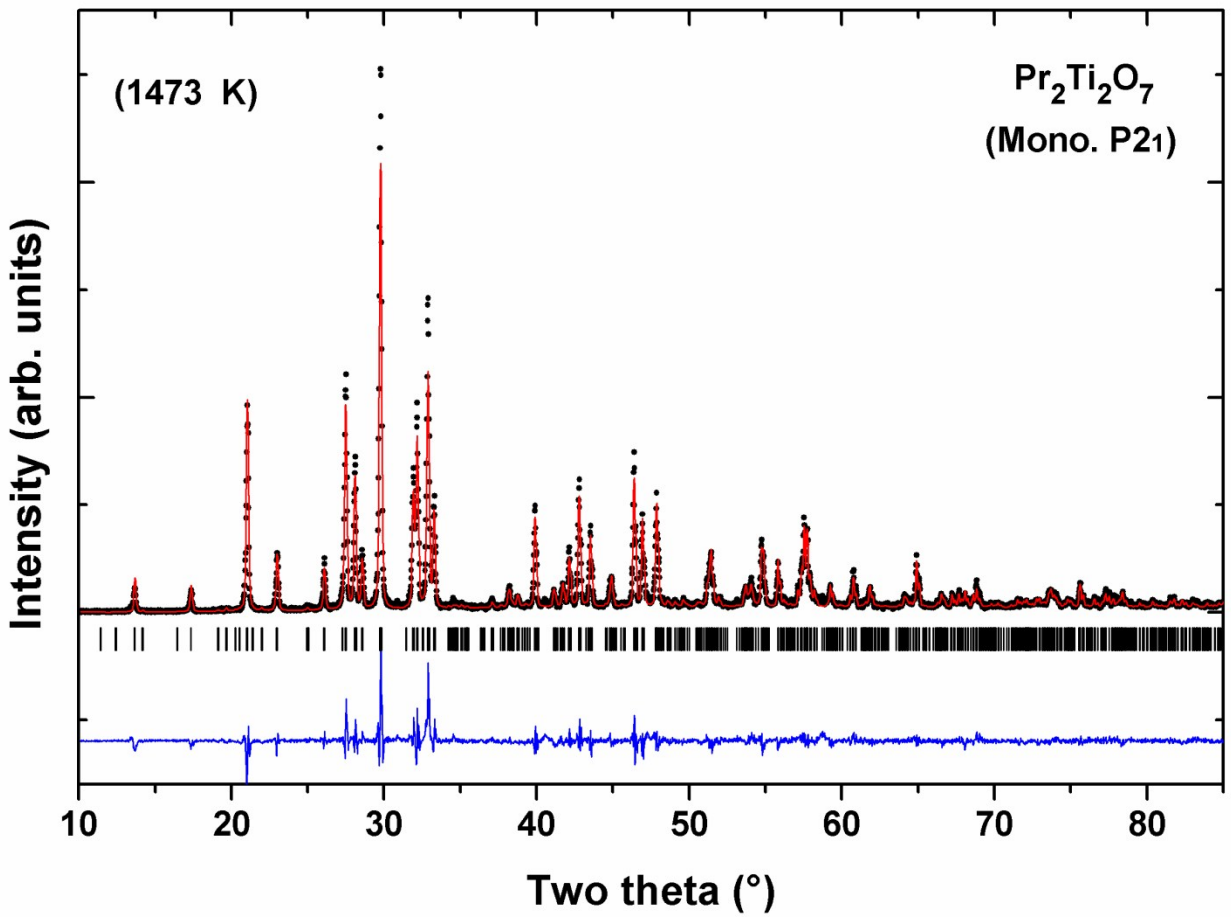
SI-IV. *UV-Vis* Diffuse reflectance spectrum of PTO.



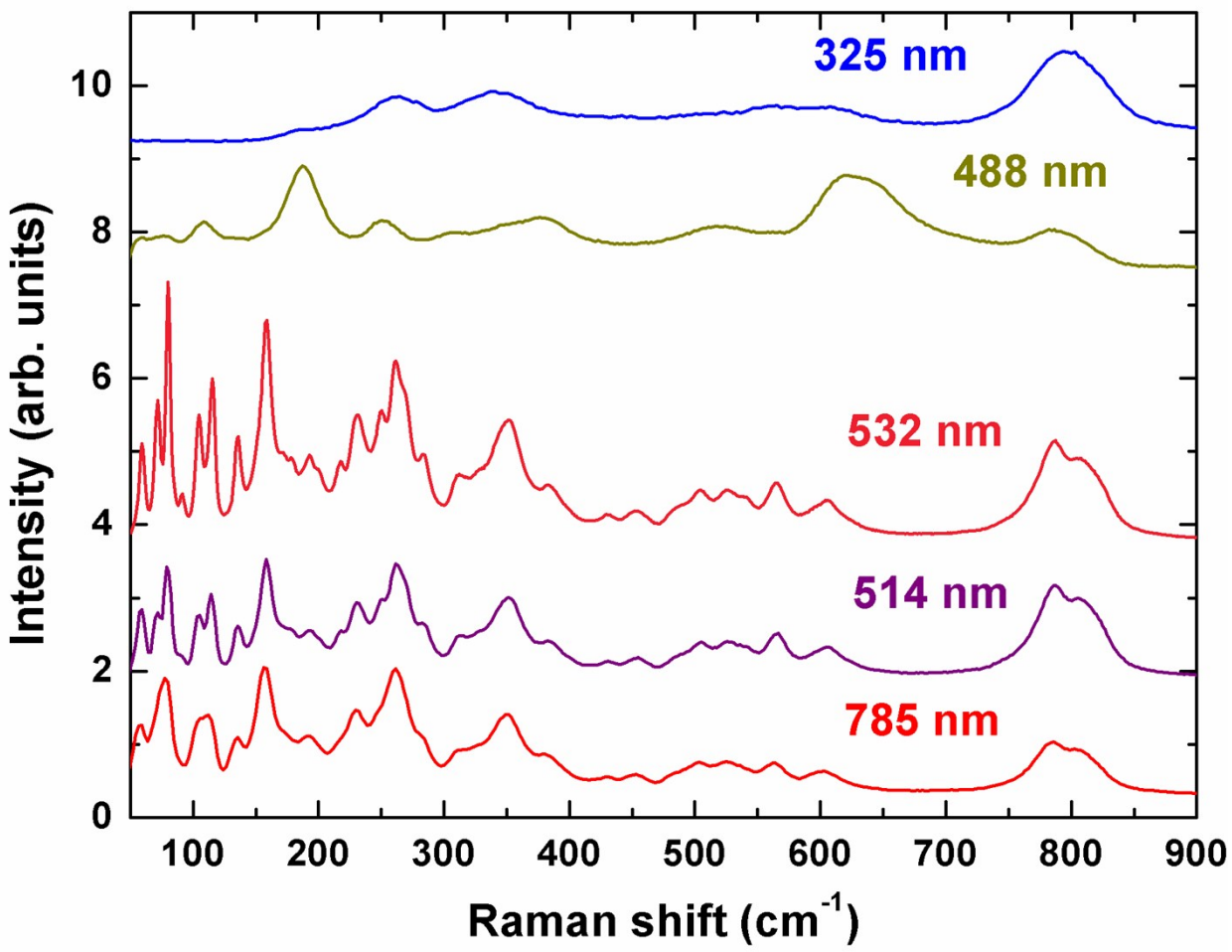
SI-V. DSC traces of PTO.



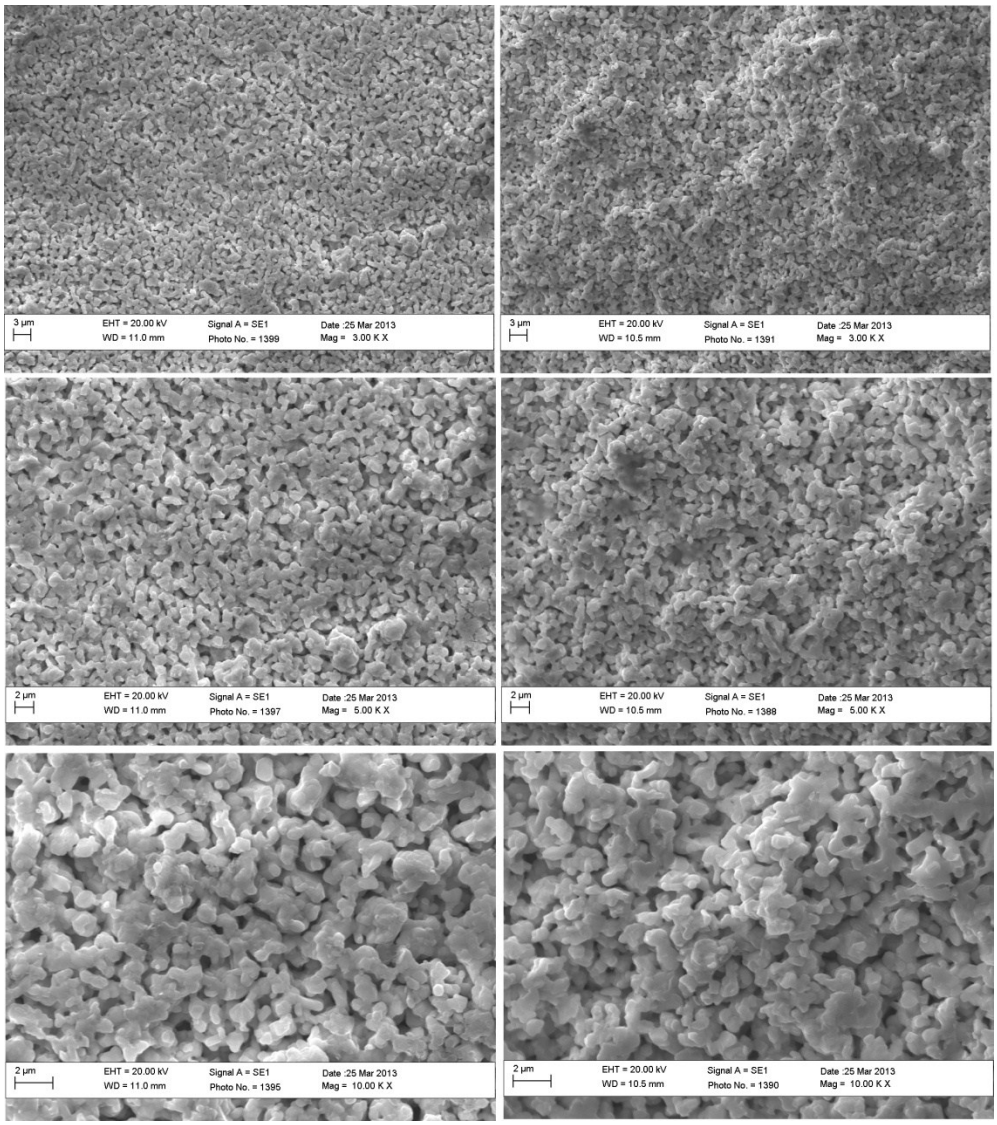
SI-VI. Rietveld refinement plot of powder XRD data of PTO recorded at 1473 K.



SI-VII. Raman spectra of PTO recorded at different excitation wavelengths.



SI-VIII. SEM images of sintered PTO pellet (Left column: Top surface; right column: Fractured surface).



SI-IX. Typical fittings of ε” of PTO withHavriliak-Negami (H-N) model.