New Mixed Metal Selenites and Tellurites Containing Pd^{2+} Ions in a Square Planar Geometry

Su-Yu Zhang,[a, b] Chun-Li Hu,[a] Jiang-Gao Mao*,[a]

Supporting information

Table S1. State Energies (eV) of the L-CB and the H-VB of the title compounds.

Scheme S1. The coordination environments around Ba(II) in $BaPd(SeO_3)_2$ (a), Bi(III) in $Bi_2Pd(SeO_3)_4$ (b) and Pb(□) in $Pb_2Pd(SeO_3)_2Cl_2$ (c).

Figure S1. Simulated and experimental XRD powder patterns for $BaPd(SeO_3)_2$ (a), $Bi_2Pd(SeO_3)_4$ (b), $Pb_2Pd(SeO_3)_2Cl_2$ (c) and $Pb_2Pd(TeO_3)_2Cl_2$ (d).

Figure S2. IR Spectra of $BaPd(SeO_3)_2$ (a), $Bi_2Pd(SeO_3)_4$ (b), $Pb_2Pd(SeO_3)_2Cl_2$ (c), and $Pb_2Pd(TeO_3)_2Cl_2$ (d).

Figure S3. Absorption spectra for $BaPd(SeO_3)_2$ (a), $Bi_2Pd(SeO_3)_4$ (b), $Pb_2Pd(SeO_3)_2Cl_2$ (c) and $Pb_2Pd(TeO_3)_2Cl_2$ (d).

Figure S4. Optical diffuse reflectance spectra for $BaPd(SeO_3)_2$ (a), $Bi_2Pd(SeO_3)_4$ (b), $Pb_2Pd(SeO_3)_2Cl_2$ (c) and $Pb_2Pd(TeO_3)_2Cl_2$ (d).

Figure S5. The PXRD patterns of the thermal decomposition residuals for $BaPd(SeO_3)_2$.

Figure S6. The band structures of $BaPd(SeO_3)_2$, $Bi_2Pd(SeO_3)_4$ and $Pb_2Pd(QO_3)_2Cl_2$ (Q = Se, Te).

Figure S7. The total density of states and partial density of states of $BaPd(SeO_3)_2$, $Bi_2Pd(SeO_3)_4$ and $Pb_2Pd(QO_3)_2Cl_2$ (Q = Se, Te) (the Fermi level is set at 0 eV).

Cif files for the structures.

Table S1. State Energies (eV) of the L-CB and the H-VB of the title compounds.

$BaPd(SeO_3)_2$	k-point	L-CB	H-VB
(-0.500 0.000 0.500)	L	1.333601	-0.28069
(-0.500 -0.500 0.500)	M	2.051396	-0.47514
(-0.500 0.000 0.000)	A	1.321754	-0.2795
(0.000 0.000 0.000)	G	2.005804	0
(0.000 -0.500 0.500)	Z	1.333602	-0.28069
(0.000 0.000 0.500)	Y	2.040714	-0.0876
$Bi_2Pd(SeO_3)_4$	k-point	L-CB	H-VB
(0.000 0.000 0.500)	Z	1.87506	-0.06531
(0.000 0.000 0.000)	G	1.732786	-0.00947
(0.000 0.500 0.000)	Y	1.901132	-0.0588
(-0.500 0.500 0.000)	A	1.859624	-0.07155
(-0.500 0.000 0.000)	B	1.746502	0
		1.730646	-0.00661
(-0.500 0.000 0.500)	D	1.911726	-0.07887
(-0.500 0.500 0.500)	E	1.909796	-0.01988
(0.000 0.500 0.500)	C	1.911236	-0.00703
$Pb_2Pd(SeO_3)_2Cl_2$	k-point	L-CB	H-VB
(0.000 0.000 0.500)	Z	1.611028	-0.22459
(0.000 0.000 0.000)	G	1.435236	-0.27218

(0.000 0.500 0.000)	Y	1.74822	-0.17649
(-0.500 0.500 0.000)	A	1.697095	-0.23647
(-0.500 0.000 0.000)	B	1.667216	0
(-0.500 0.000 0.500)	D	1.65292	-0.22256
(-0.500 0.500 0.500)	E	1.724946	-0.13943
(0.000 0.500 0.500)	C	1.745808	-0.20726
$Pb_2Pd(TeO_3)_2Cl_2$	k-point	L-CB	H-VB
(0.000 0.000 0.500)	Z	1.692913	-0.2669
(0.000 0.000 0.000)	G	1.426912	-0.28505
(0.000 0.500 0.000)	Y	1.777802	-0.11053
(-0.500 0.500 0.000)	A	1.720093	-0.20291
(-0.500 0.000 0.000)	B	1.695195	0
(-0.500 0.000 0.500)	D	1.693771	-0.19609
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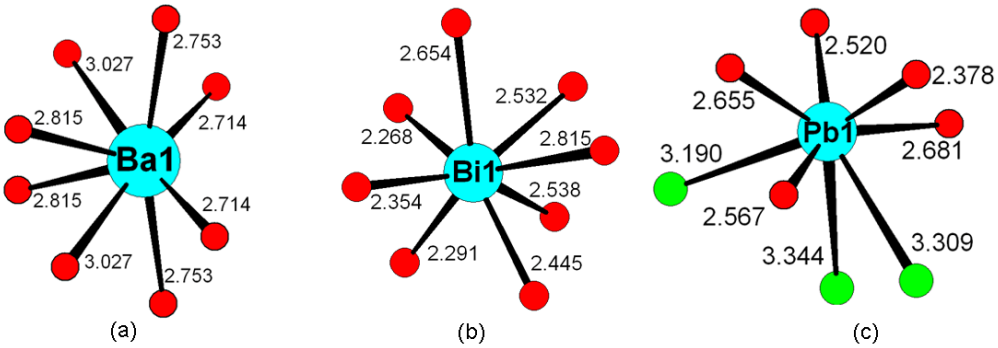
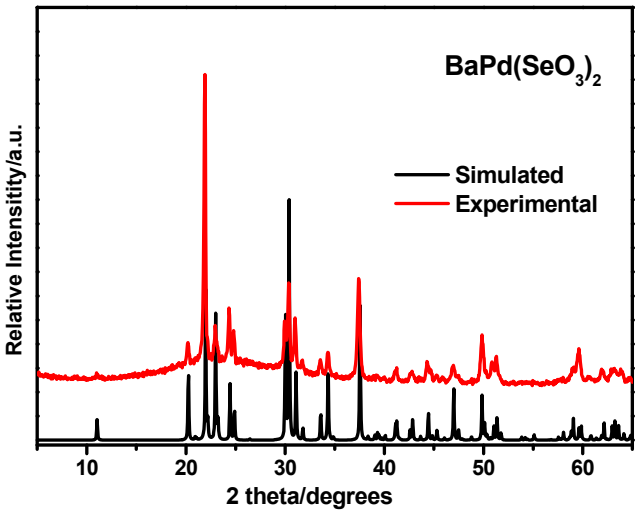


Scheme S1. The coordination environments around Ba(II) in $BaPd(SeO_3)_2$ (a), Bi(III) in $Bi_2Pd(SeO_3)_4$ (b) and Pb(□) in $Pb_2Pd(SeO_3)_2Cl_2$ (c).



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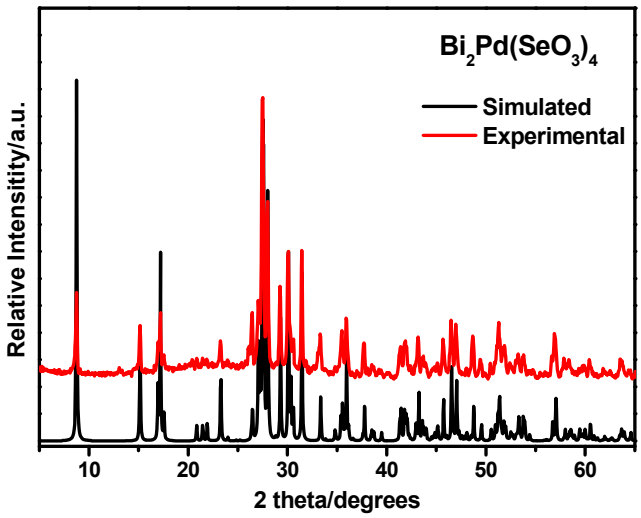

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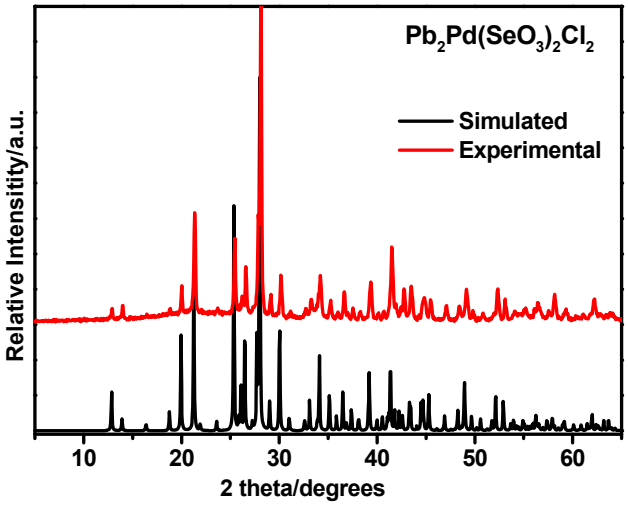

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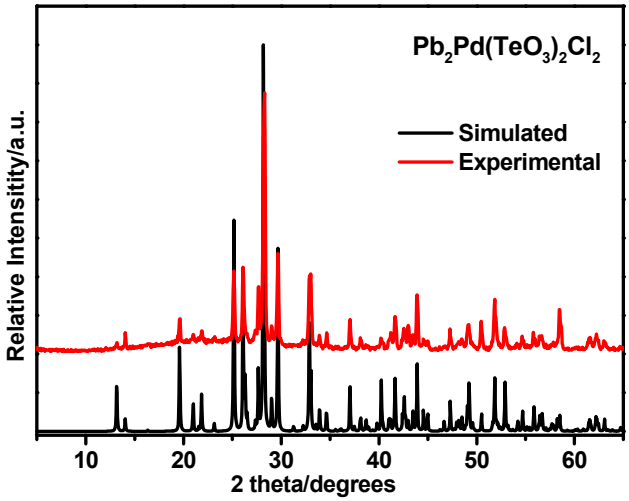

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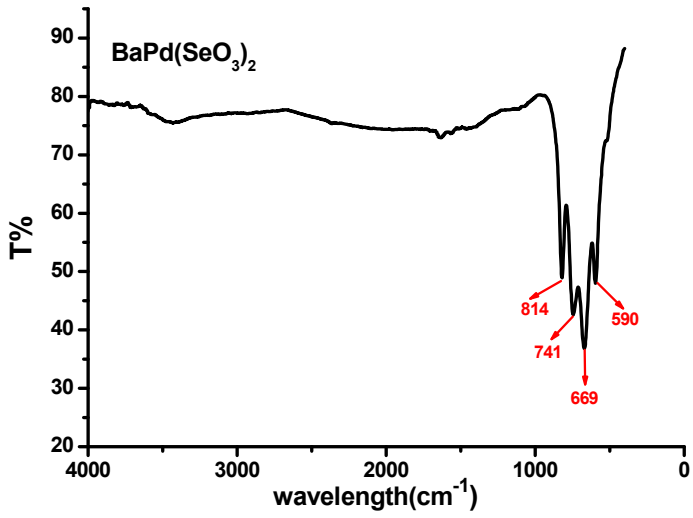
Figure S1. Simulated and experimental XRD powder patterns for $BaPd(SeO_3)_2$ (a), $Bi_2Pd(SeO_3)_4$ (b), $Pb_2Pd(SeO_3)_2Cl_2$ (c) and $Pb_2Pd(TeO_3)_2Cl_2$ (d).



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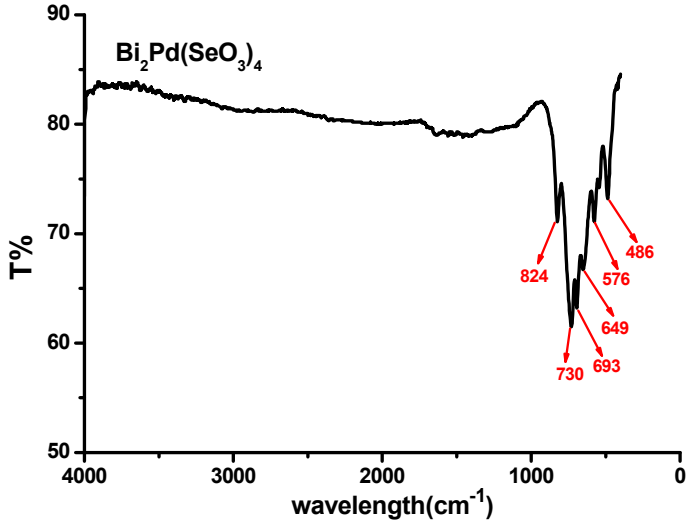

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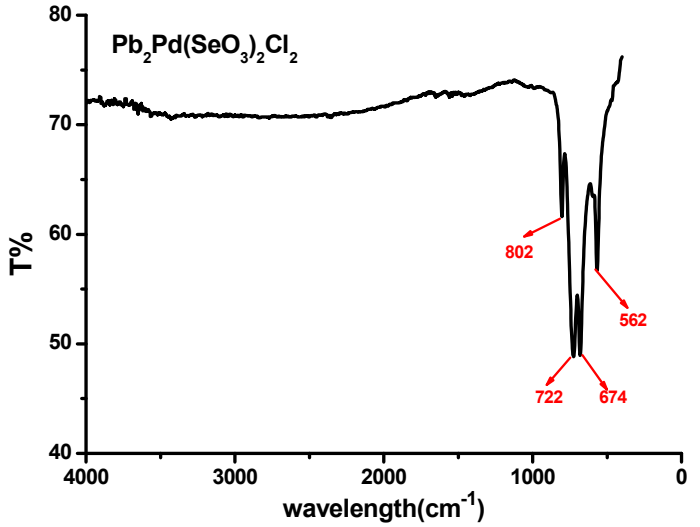

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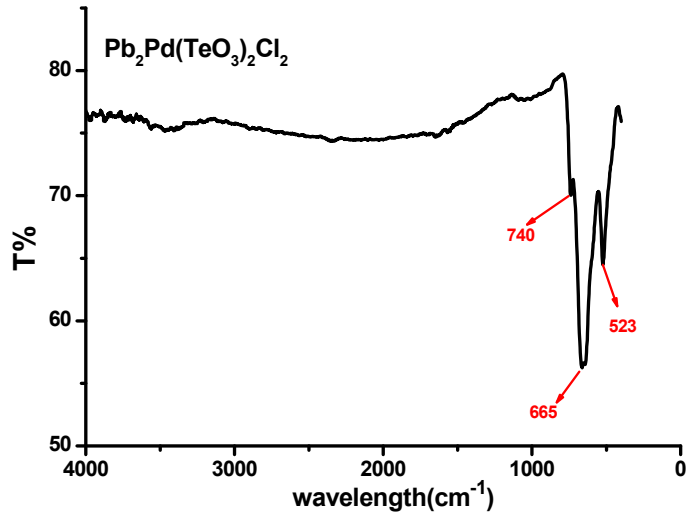

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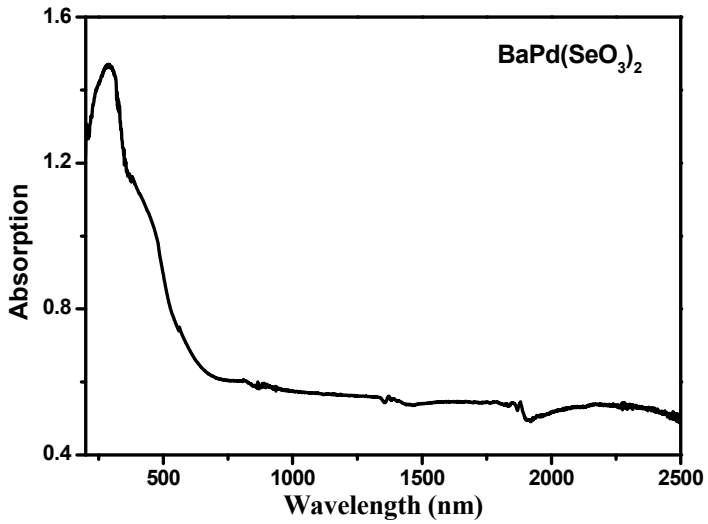
Figure S2. IR Spectra of $BaPd(SeO_3)_2$ (a), $Bi_2Pd(SeO_3)_4$ (b), $Pb_2Pd(SeO_3)_2Cl_2$ (c), and $Pb_2Pd(TeO_3)_2Cl_2$ (d).



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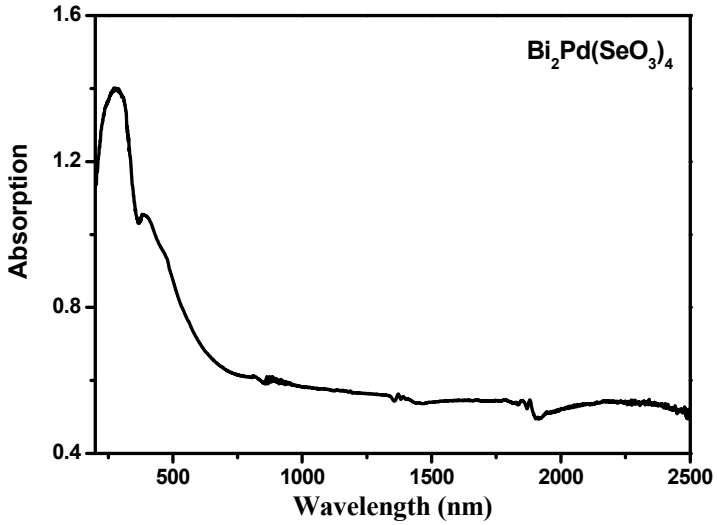

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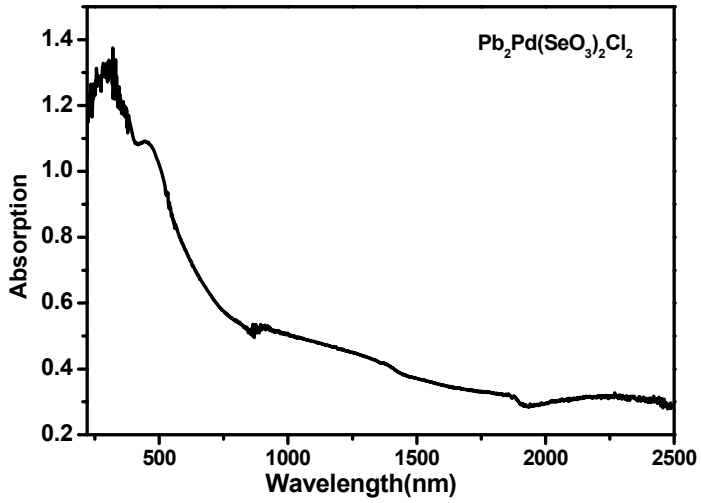

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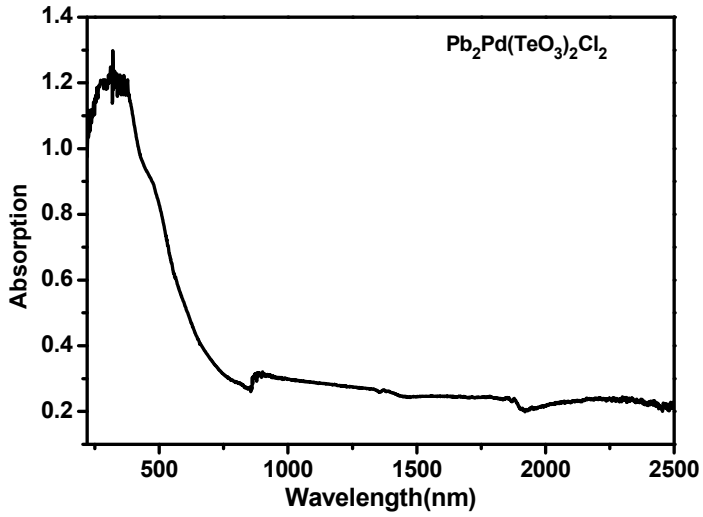

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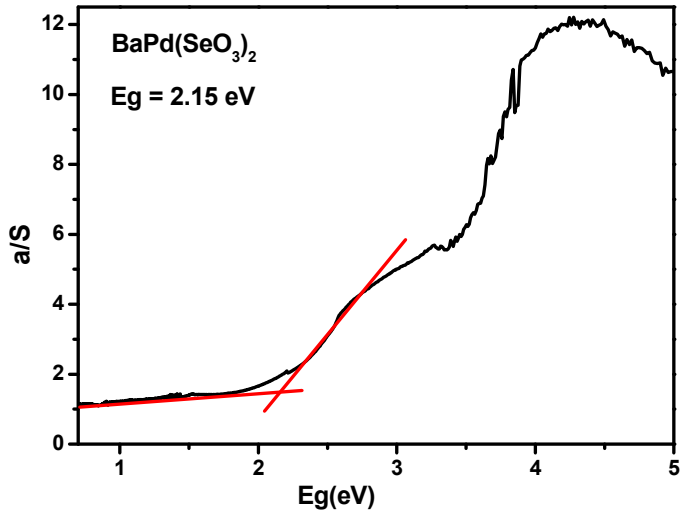
Figure S3. Absorption spectra for $BaPd(SeO_3)_2$ (a), $Bi_2Pd(SeO_3)_4$ (b), $Pb_2Pd(SeO_3)_2Cl_2$ (c) and $Pb_2Pd(TeO_3)_2Cl_2$ (d).



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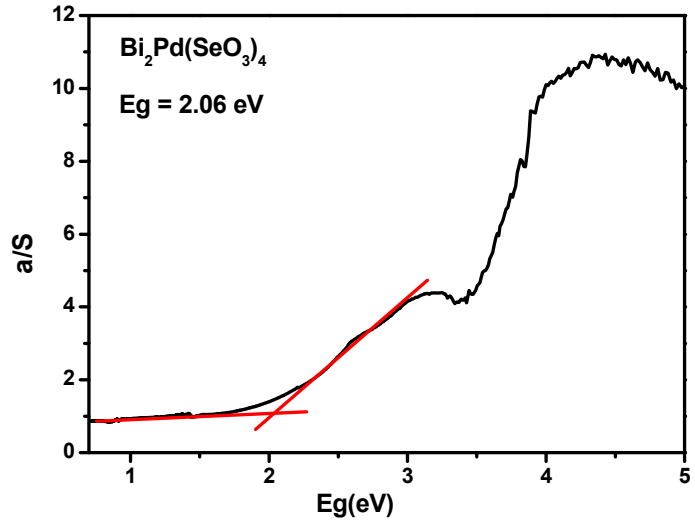

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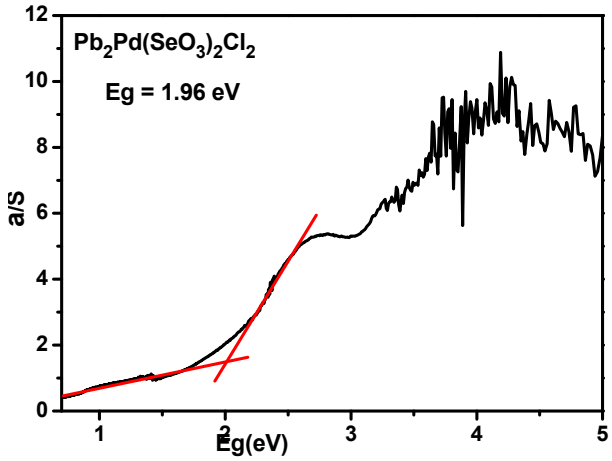

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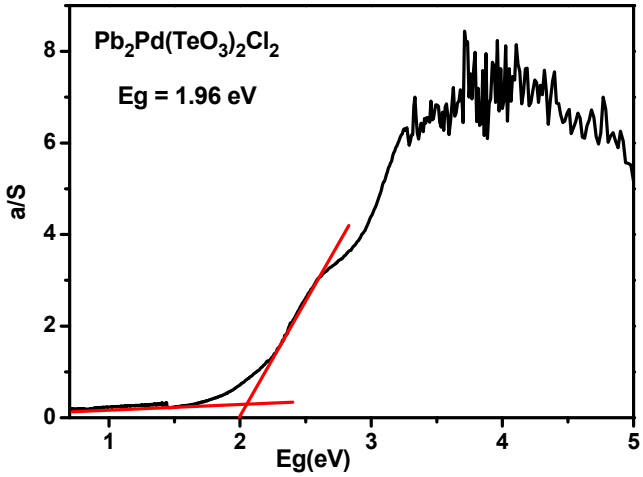

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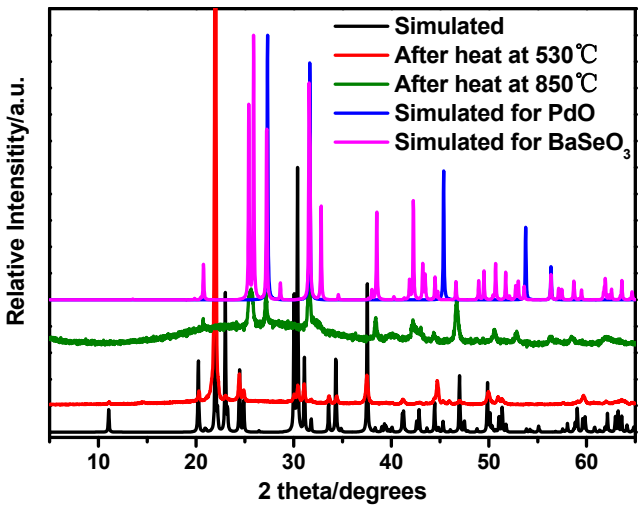

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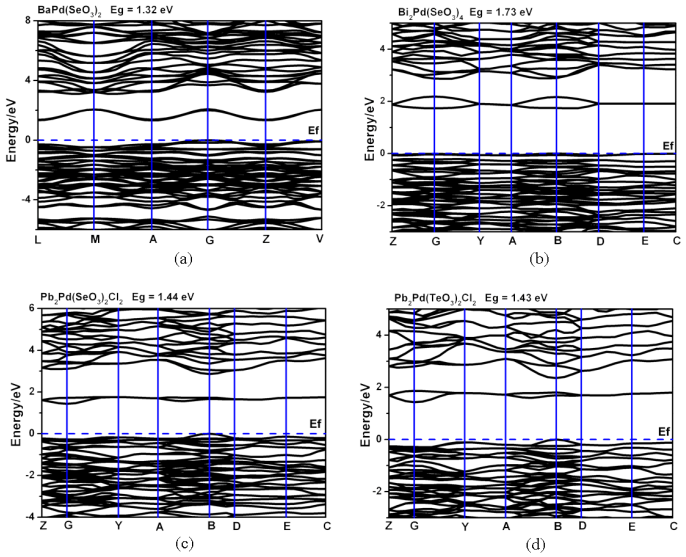

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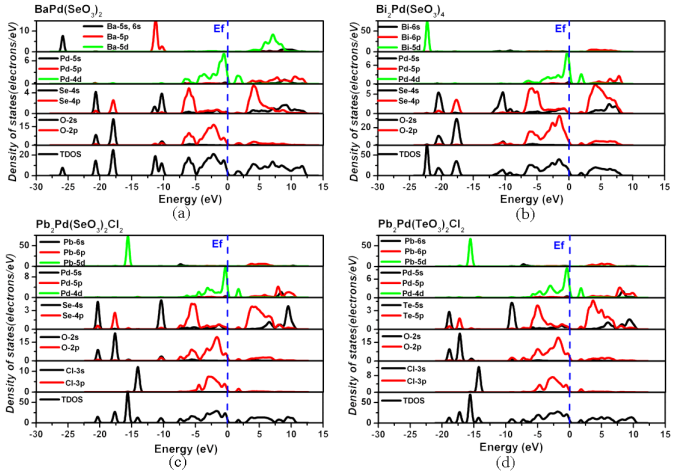

Figure S7. The total density of states and partial density of states of $BaPd(SeO_3)_2$, $Bi_2Pd(SeO_3)_4$ and $Pb_2Pd(QO_3)_2Cl_2$ (Q = Se, Te) (the Fermi level is set at 0 eV).

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;
Higashi, T. (1995). Program for Absorption Correction.
Rigaku Corporation, Tokyo, Japan.
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Refinement of F^2^ against ALL reflections. The weighted R-factor wR and
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F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
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on F^2^ are statistically about twice as large as those based on F, and R-
factors based on ALL data will be even larger.
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are estimated using the full covariance matrix. The cell esds are taken
into account individually in the estimation of esds in distances, angles
and torsion angles; correlations between esds in cell parameters are only
used when they are defined by crystal symmetry. An approximate (isotropic)
treatment of cell esds is used for estimating esds involving l.s. planes.
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Pb1 Cl1 Pb1 118.37(8) . 2_445 ?
Pb1 Cl1 Pb1 115.05(8) 1_545 2_445 ?
Se1 O1 Pb1 125.6(3) . . ?
Se1 O1 Pb1 103.6(3) . 2 ?
Pb1 O1 Pb1 130.7(3) . 2 ?
Se1 O2 Pd1 126.0(4) . . ?
Se1 O2 Pb1 107.0(3) . 2 ?

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Pd Pd -0.9988 1.0072 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
Bi Bi -4.1077 10.2566 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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'x, -y-1/2, z-1/2'

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Higashi, T. (1995). Program for Absorption Correction.
Rigaku Corporation, Tokyo, Japan.
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Refinement of F^2^ against ALL reflections. The weighted R-factor wR and
goodness of fit S are based on F^2^, conventional R-factors R are based
on F, with F set to zero for negative F^2^. The threshold expression of
F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
not relevant to the choice of reflections for refinement. R-factors based
on F^2^ are statistically about twice as large as those based on F, and R-
factors based on ALL data will be even larger.
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Pd1 Pd -0.5000 0.0000 1.0000 0.00584(13) Uani 1 2 d S . .
Se1 Se -0.18655(5) 0.17301(7) 0.86216(6) 0.00477(12) Uani 1 1 d . . .
Se2 Se -0.36518(5) -0.16733(7) 0.38706(6) 0.00600(12) Uani 1 1 d . . .
O1 O -0.3429(4) -0.0971(5) 0.1953(4) 0.0084(8) Uani 1 1 d . . .
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O3 O -0.0729(4) 0.3548(4) 0.9175(4) 0.0068(8) Uani 1 1 d . . .
O4 O -0.4375(4) -0.3771(5) 0.3190(5) 0.0116(9) Uani 1 1 d . . .
O5 O -0.0940(4) 0.0119(5) 0.8052(5) 0.0080(8) Uani 1 1 d . . .
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Se2 0.0051(3) 0.0071(3) 0.0050(2) 0.00119(19) 0.0008(2) 0.0010(2)
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O2 0.009(2) 0.0059(18) 0.0068(17) 0.0017(14) 0.0024(16) 0.0033(15)
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All esds (except the esd in the dihedral angle between two l.s. planes)
are estimated using the full covariance matrix. The cell esds are taken
into account individually in the estimation of esds in distances, angles
and torsion angles; correlations between esds in cell parameters are only
used when they are defined by crystal symmetry. An approximate (isotropic)
treatment of cell esds is used for estimating esds involving l.s. planes.
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Bi1 O3 2.660(4) 4_565 ?
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O2 Bi1 O6 78.10(12) 3_557 2_556 ?
O3 Bi1 O6 148.10(12) 2_546 2_556 ?
O5 Bi1 O6 98.87(13) . 2_556 ?
O2 Bi1 O1 70.68(12) 3_557 3_556 ?
O3 Bi1 O1 86.68(12) 2_546 3_556 ?
O5 Bi1 O1 147.91(12) . 3_556 ?
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O5 Se1 O3 99.09(18) . . ?
O2 Se1 O3 96.74(17) . . ?
O6 Se2 O4 104.72(18) . . ?
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Bi1 O3 Bi1 115.15(13) 2_556 4_566 ?
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Pd Pd -0.9988 1.0072 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
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'-x+1/2, -y+1/2, -z'
'x+1/2, -y+1/2, z-1/2'

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Rigaku Corporation, Tokyo, Japan.
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Refinement of F^2^ against ALL reflections. The weighted R-factor wR and
goodness of fit S are based on F^2^, conventional R-factors R are based
on F, with F set to zero for negative F^2^. The threshold expression of
F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
not relevant to the choice of reflections for refinement. R-factors based
on F^2^ are statistically about twice as large as those based on F, and R-
factors based on ALL data will be even larger.
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Se1 Se 0.13035(7) 0.00696(9) 0.09372(3) 0.00670(15) Uani 1 1 d . . .
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All esds (except the esd in the dihedral angle between two l.s. planes)
are estimated using the full covariance matrix. The cell esds are taken
into account individually in the estimation of esds in distances, angles
and torsion angles; correlations between esds in cell parameters are only
used when they are defined by crystal symmetry. An approximate (isotropic)
treatment of cell esds is used for estimating esds involving l.s. planes.
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