Syntheses and crystal structures of four new silver(I) iodates with d^0-transition metal cations

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Supporting Information

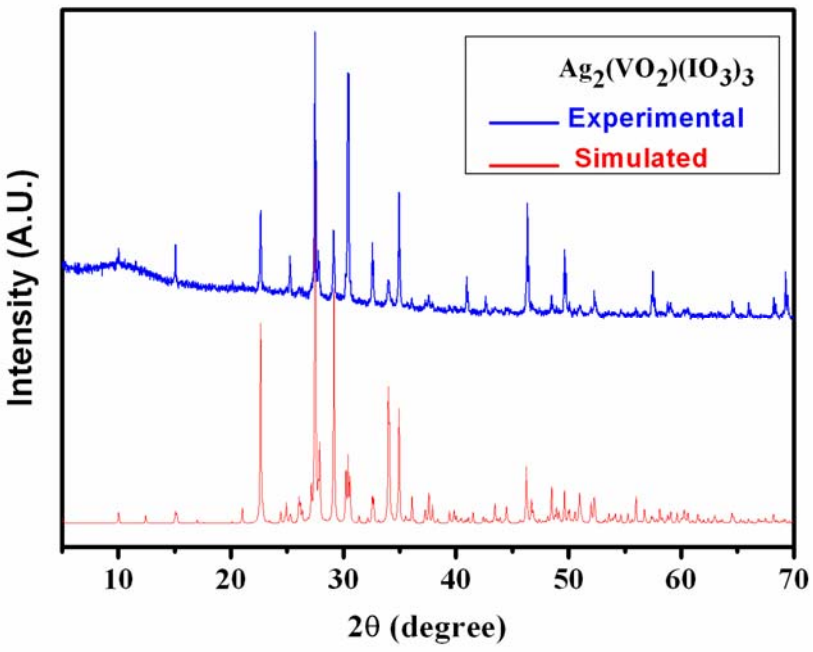
Table S1. The state energies (eV) of the lowest conduction band (L-CB) and the highest valence band (H-VB) of the compounds.

Compound	k-point	L-CB	H-VB
$Ag_2Ti(IO_3)_6$	F (0.500, 0.000, -0.500)	2.63354	-0.06517
	G (0.000, 0.000, 0.000)	3.11124	-0.00977
	Z (0.500, 0.500, -0.500)	2.74795	-0.1009
$Ag_2(VO_2)(IO_3)_3$	G (0.000, 0.000, 0.000)	1.73235	0
	Z (0.000, 0.000, 0.500)	1.86021	-0.12211
	T (-0.500, 0.000, 0.500)	1.86028	-0.1245
	Y (-0.500, 0.000, 0.000)	1.73259	-0.00427
	S (-0.500, 0.500, 0.000)	1.76454	-0.01764
	X (0.000, 0.500, 0.000)	1.76424	-0.01732
	U (0.000, 0.500, 0.500)	1.81258	-0.20866
	R (-0.500, 0.500, 0.500)	1.81265	-0.21059
$Ag_2(V_2O_4)(IO_3)_4$	G (0.000, 0.000, 0.000)	2.15024	-0.00891
	Z (0.000, 0.000, 0.500)	2.15746	-0.0313
	T (-0.500, 0.000, 0.500)	2.16355	-0.04238
	Y (-0.500, 0.000, 0.000)	2.17405	-0.00556
	S (-0.500, 0.500, 0.000)	2.17466	0
	X (0.000, 0.500, 0.000)	2.17363	-0.00868
	U (0.000, 0.500, 0.500)	2.18236	-0.0273
	R (-0.500, 0.500, 0.500)	2.17896	-0.01311
$Ag_2(MoO_2)(IO_3)_4$	L (-0.500, 0.000, 0.500)	2.30048	-0.112
	M (-0.500, -0.500, 0.500)	2.37752	0
	A (-0.500, 0.000, 0.000)	2.17908	-0.11929
	G (0.000, 0.000, 0.000)	2.23341	-0.27318
	Z (0.000, -0.500, 0.500)	2.30048	-0.112
	V (0.000, 0.000, 0.500)	2.23891	-0.30068

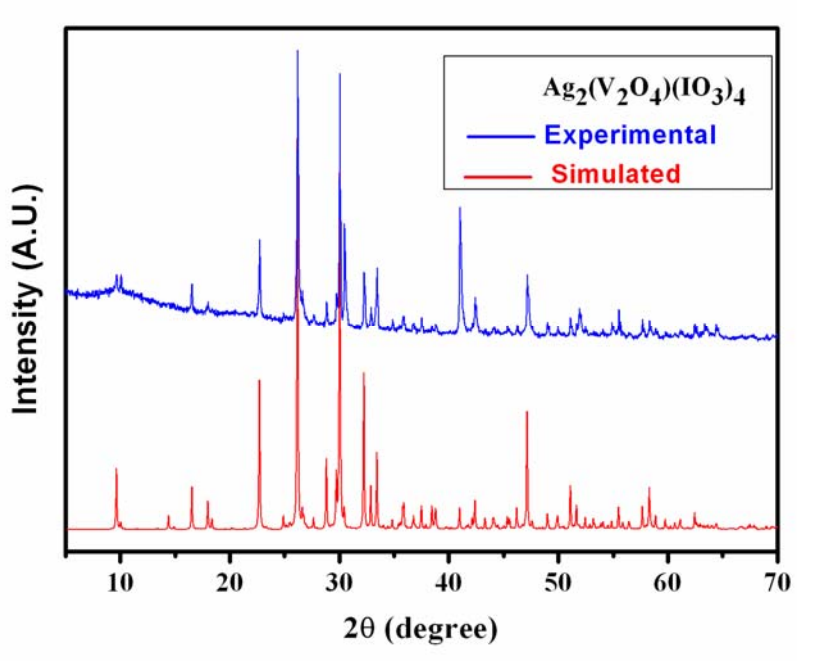
Table S2. The calculated bond orders of the compounds.

For $Ag_2Ti(IO_3)_6$					
Bond	Bond length	Bond order	Bond	Bond length	Bond order
Ti-O	1.946	0.47	I-O	1.810	0.39
I-O	1.813	0.42	I-O	1.885	0.21
Ag-O	2.563	0.14	Ag-O	2.810	0.05
For $Ag_2(VO_2)(IO_3)_3$					
Bond	Bond length	Bond order	Bond	Bond length	Bond order
V-O	1.605	0.95	V-O	1.706	0.77
V-O	1.907	0.48	V-O	2.022	0.33
V-O	2.058	0.35	V-O	2.431	0.13
I-O	1.778	0.46	I-O	1.797	0.37
I-O	1.798	0.34	I-O	1.810	0.43
I-O	1.816	0.31	I-O	1.818	0.38
I-O	1.827	0.28	I-O	1.849	0.24
I-O	1.910	0.18	Ag-O	2.311	0.18
Ag-O	2.344	0.16	Ag-O	2.365	0.15
Ag-O	2.367	0.17	Ag-O	2.452	0.12
Ag-O	2.546	0.10	Ag-O	2.723	0.06
Ag-O	2.727	0.06	Ag-O	2.793	0.06
Ag-O	2.833	0.04	Ag-O	2.841	0.03
For $Ag_2(V_2O_4)(IO_3)_4$					
Bond	Bond length	Bond order	Bond	Bond length	Bond order
V-O	1.602	0.94	V-O	1.624	0.90
V-O	1.676	0.77	V-O	1.698	0.75
V-O	1.958	0.39	V-O	1.985	0.38
V-O	1.998	0.35	V-O	2.001	0.35
V-O	2.069	0.30	V-O	2.098	0.32
V-O	2.202	0.20	V-O	2.222	0.22
I-O	1.791	0.42	I-O	1.797	0.40
I-O	1.804	0.39	I-O	1.811	0.35
I-O	1.813	0.42	I-O	1.820	0.36
I-O	1.831	0.30	I-O	1.834	0.27
I-O	1.834	0.29	I-O	1.852	0.26
I-O	1.854	0.22	I-O	1.863	0.21
Ag-O	2.461	0.12	Ag-O	2.484	0.12
Ag-O	2.496	0.11	Ag-O	2.507	0.10
Ag-O	2.529	0.08	Ag-O	2.540	0.11
Ag-O	2.549	0.11	Ag-O	2.564	0.10
Ag-O	2.571	0.09	Ag-O	2.593	0.09
Ag-O	2.611	0.08	Ag-O	2.668	0.06
For $Ag_2(MoO_2)(IO_3)_4$					
Bond	Bond length	Bond order	Bond	Bond length	Bond order

Mo-O	1.716	0.93	Mo-O	1.955	0.47
Mo-O	2.199	0.25	I-O	1.798	0.40
I-O	1.805	0.40	I-O	1.832	0.38
I-O	1.809	0.30	I-O	1.850	0.27
I-O	1.917	0.15	Ag-O	2.410	0.12
Ag-O	2.448	0.15	Ag-O	2.541	0.08
Ag-O	2.602	0.09	Ag-O	2.630	0.07
Ag-O	2.640	0.10			



(a)



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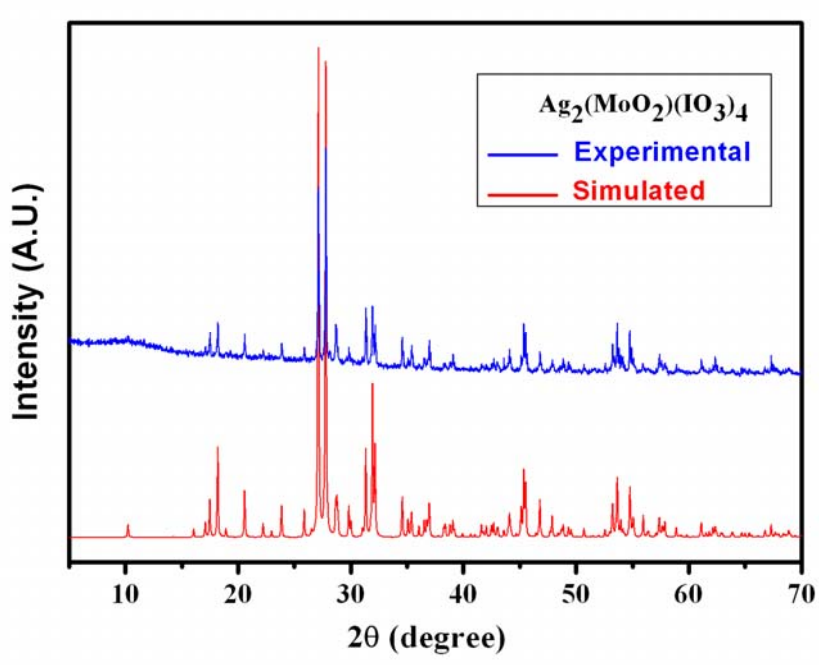
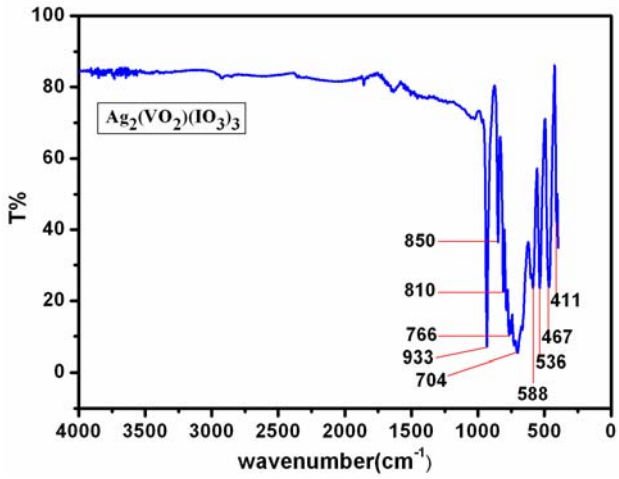
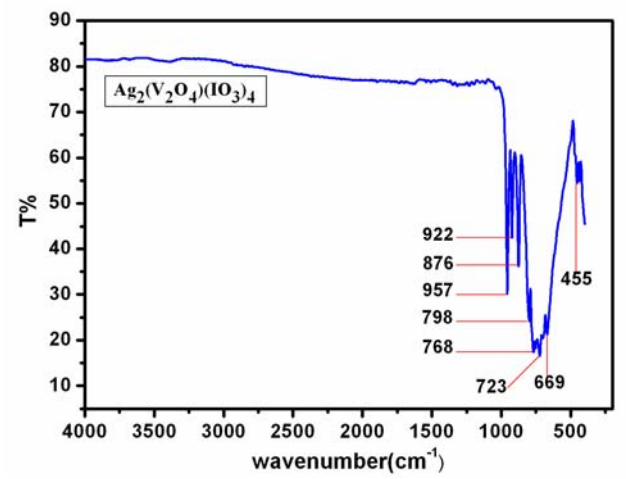


(c)

Figure S1. Simulated and experimental XRD powder patterns for $Ag_2(VO_2)(IO_3)_3$, $Ag_2(V_2O_4)(IO_3)_4$, and $Ag_2(MoO_2)(IO_3)_4$.



(a)



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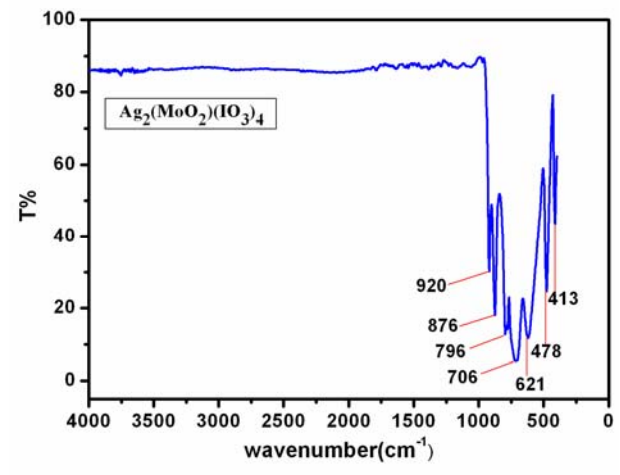

(c)

Figure S2. IR spectra for $Ag_2(VO_2)(IO_3)_3$ (a), $Ag_2(V_2O_4)(IO_3)_4$ (b), and $Ag_2(MoO_2)(IO_3)_4$ (c).

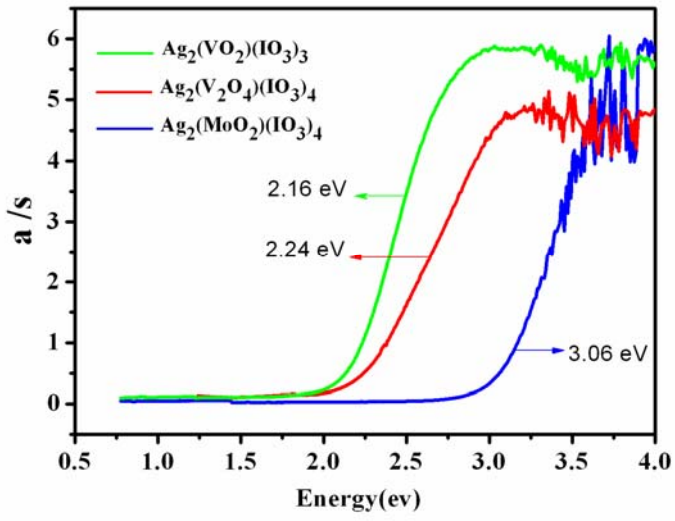

Figure S3. Optical diffuse reflectance spectra for $Ag_2(VO_2)(IO_3)_3$, $Ag_2(V_2O_4)(IO_3)_4$,

and $Ag_2(MoO_2)(IO_3)_4$.

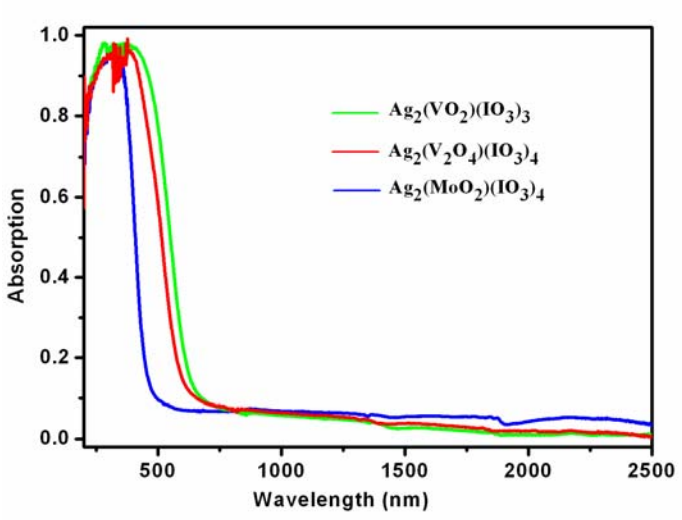

Figure S4. UV absorption spectra for $Ag_2(VO_2)(IO_3)_3$, $Ag_2(V_2O_4)(IO_3)_4$, and $Ag_2(MoO_2)(IO_3)_4$.

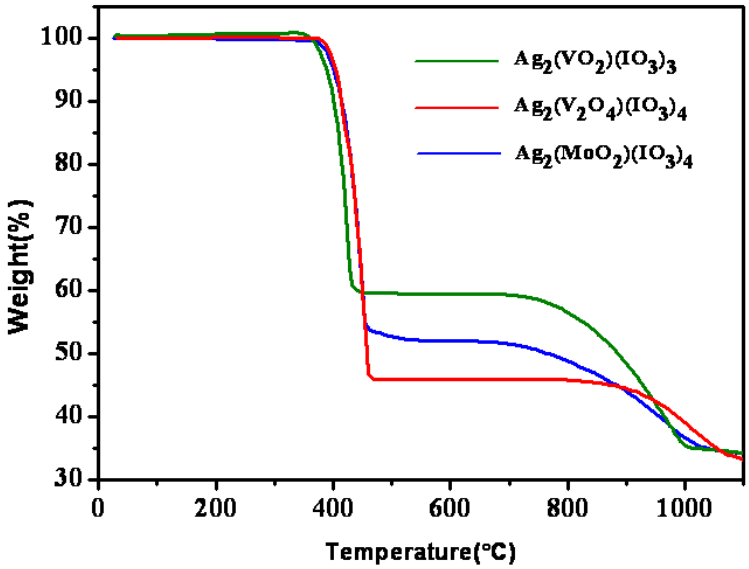

Figure S5. TGA curves for $Ag_2(VO_2)(IO_3)_3$, $Ag_2(V_2O_4)(IO_3)_4$, and $Ag_2(MoO_2)(IO_3)_4$.

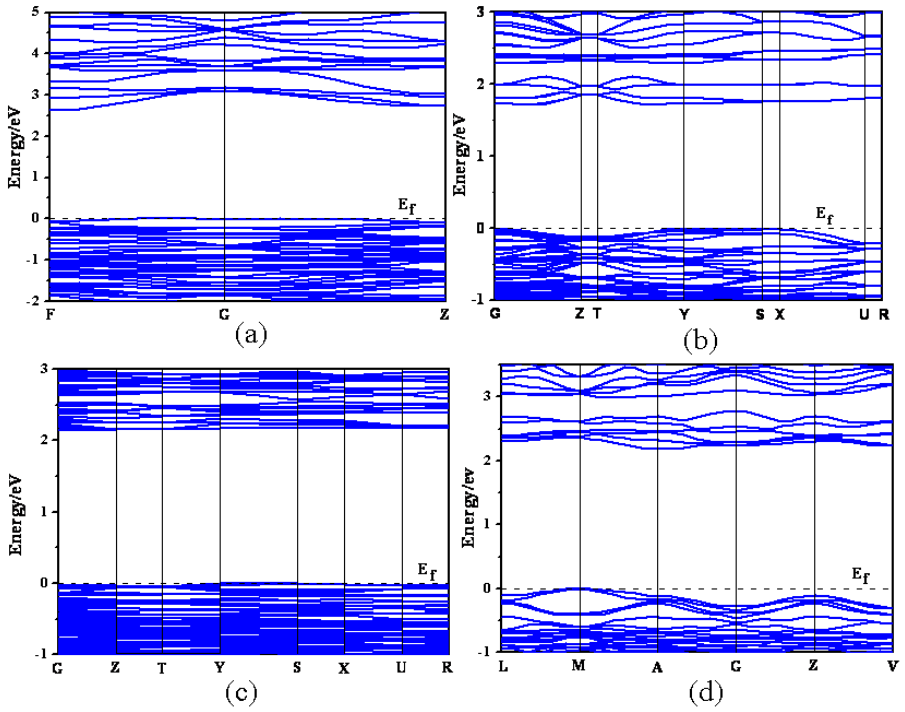

Figure S6. Band structures for $Ag_2Ti(IO_3)_6$ (a), $Ag_2(VO_2)(IO_3)_3$ (b), $Ag_2(V_2O_4)(IO_3)_4$ (c), and $Ag_2(MoO_2)(IO_3)_4$ (d). The Fermi level is set at 0 eV.

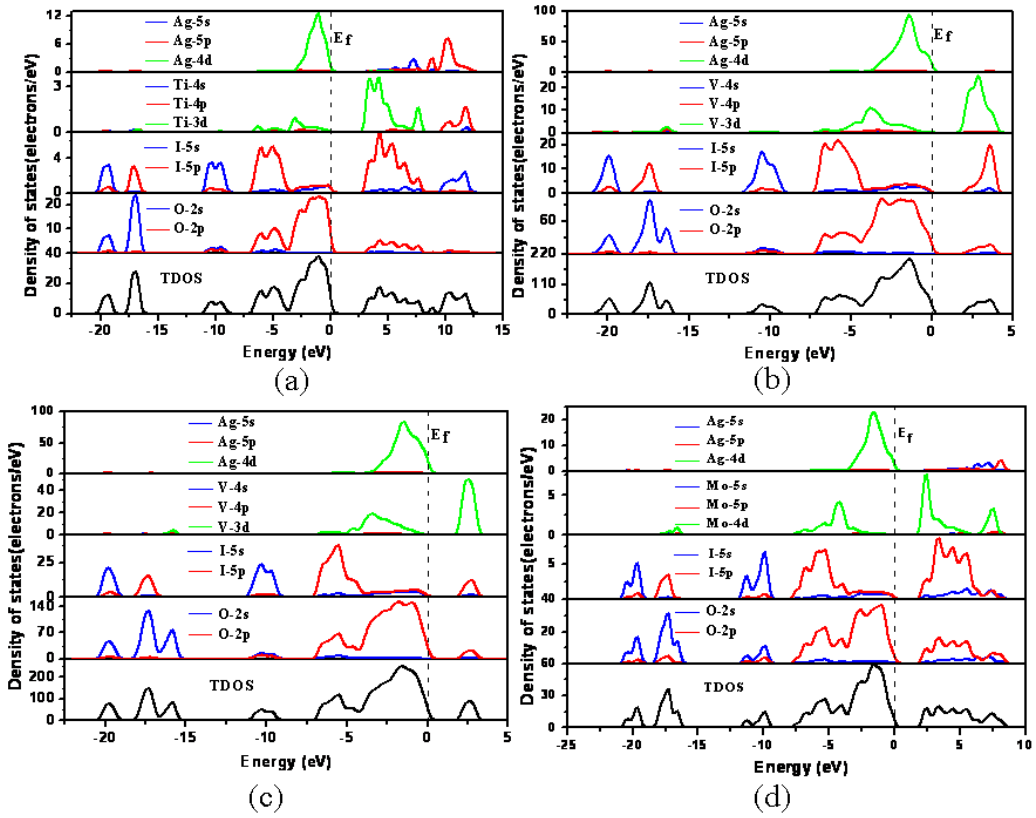

Figure S7. Total and partial density of states of $Ag_2Ti(IO_3)_6$ (a), $Ag_2(VO_2)(IO_3)_3$ (b), $Ag_2(V_2O_4)(IO_3)_4$ (c), and $Ag_2(MoO_2)(IO_3)_4$ (d). The Fermi level is set at 0 eV.