

A Series of Novel Silver Selenites with d⁰-TM Cations

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Table S1. Calculated dipole moments for all asymmetric units and the unit cells in

$\text{Ag}_3\text{Ti}_3\text{O}_3(\text{SeO}_3)_4\text{F}$ (D = Debyes).

Figure S1. Simulated and experimental XRD powder patterns of **1** (a), **2** (b), **3** (c) and **4**(d).

Figure S2. TGA and DTA curves of compounds **1**(a), **2**(b), **3**(c) and **4**(d).

Figure S3. IR spectra of compounds **1**(a), **2**(b), **3**(c) and **4**(d).

Figure S4. UV-Vis-NIR Diffuse Reflectance spectra of compounds **1**(a), **2**(b), **3**(c) and **4**(d).

Table S1. Calculated dipole moments for all asymmetric units and the unit cells in $\text{Ag}_3\text{Ti}_3\text{O}_3(\text{SeO}_3)_4\text{F}$ (D = Debyes)

	Species	dipole moment (D)			
		total	x	y	z
$\text{Ag}_3\text{Ti}_3\text{O}_3(\text{SeO}_3)_4\text{F}$	Ti(1)O ₆	4.073	3.736	-1.501	0.616
		4.073	-3.168	-2.485	0.616
		4.073	-0.569	3.986	0.616
		4.073	0.568	-3.986	0.616
		4.073	3.167	2.485	0.616
		4.073	-3.736	1.501	0.616
	Se(1)O ₃	9.668	8.620	4.302	0.816
		9.668	-8.035	5.314	0.816
		9.669	-0.585	-9.617	0.816
		9.668	0.584	9.616	0.816
		9.668	8.036	-5.314	0.816
		9.668	-8.620	-4.302	0.816
	Se(2)O ₃	9.374	0	0	9.374
		9.374	0	0	9.374
	Net(unit cell)	27.33	0	0	27.33

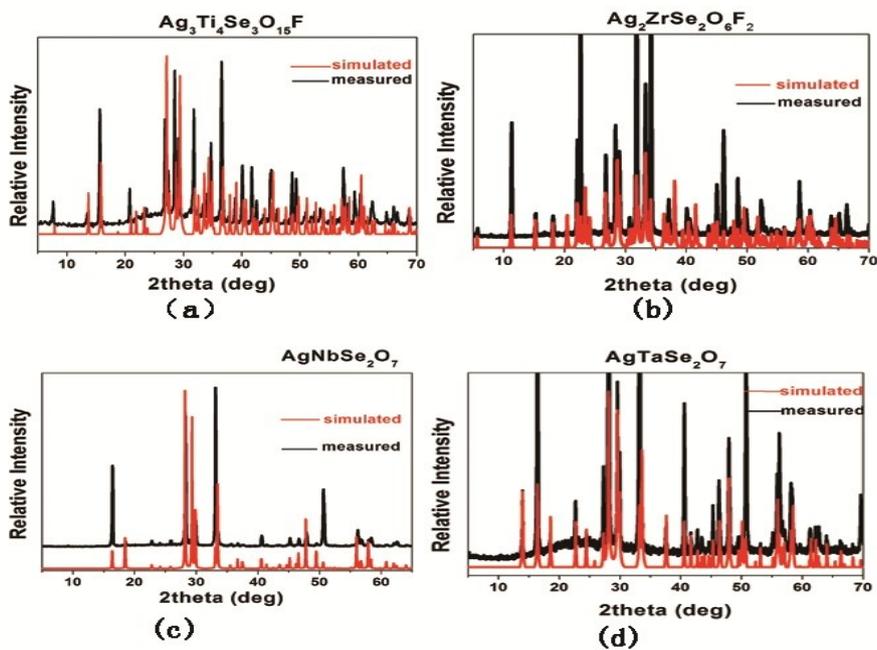


Figure S1. Simulated and experimental XRD powder patterns of **1** (a), **2** (b), **3** (c) and **4**(d).

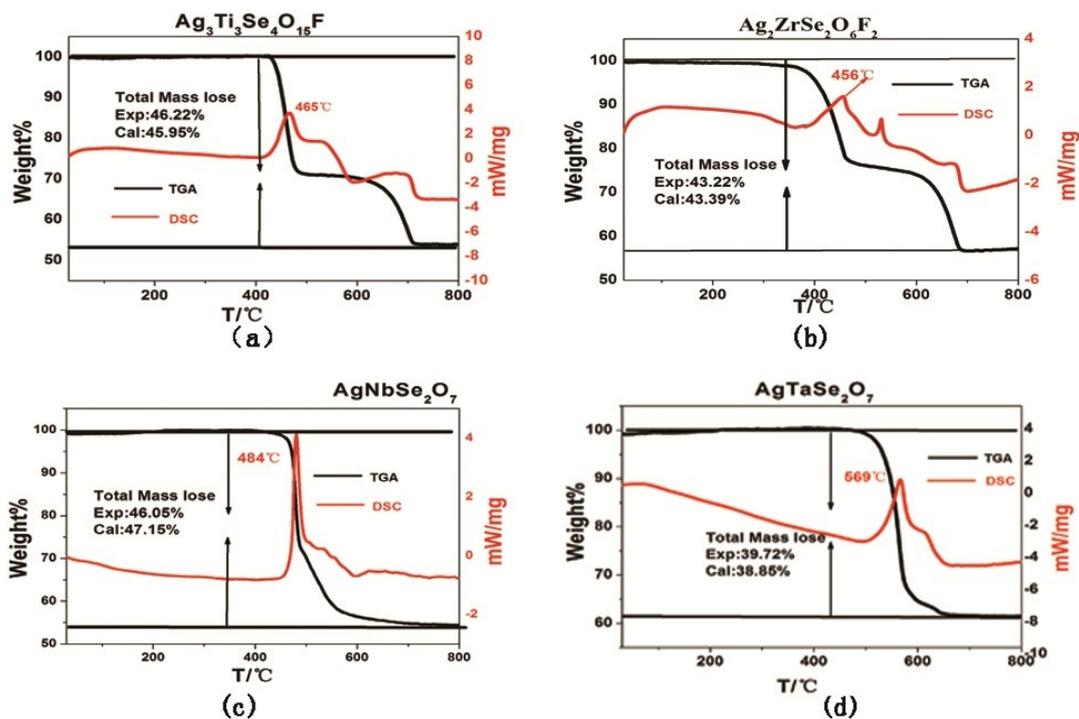


Figure S2. TGA and DTA curves of compounds 1(a), 2(b), 3(c) and 4(d).

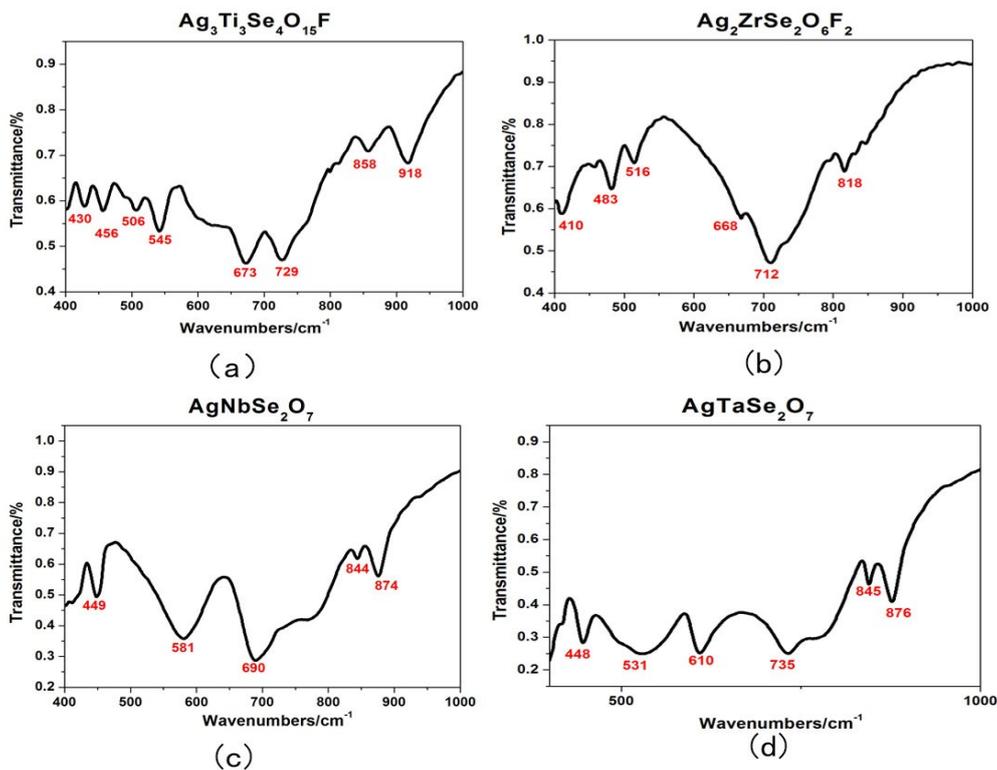


Figure S3. IR spectra of compounds **1(a)**, **2(b)**, **3(c)** and **4(d)**.

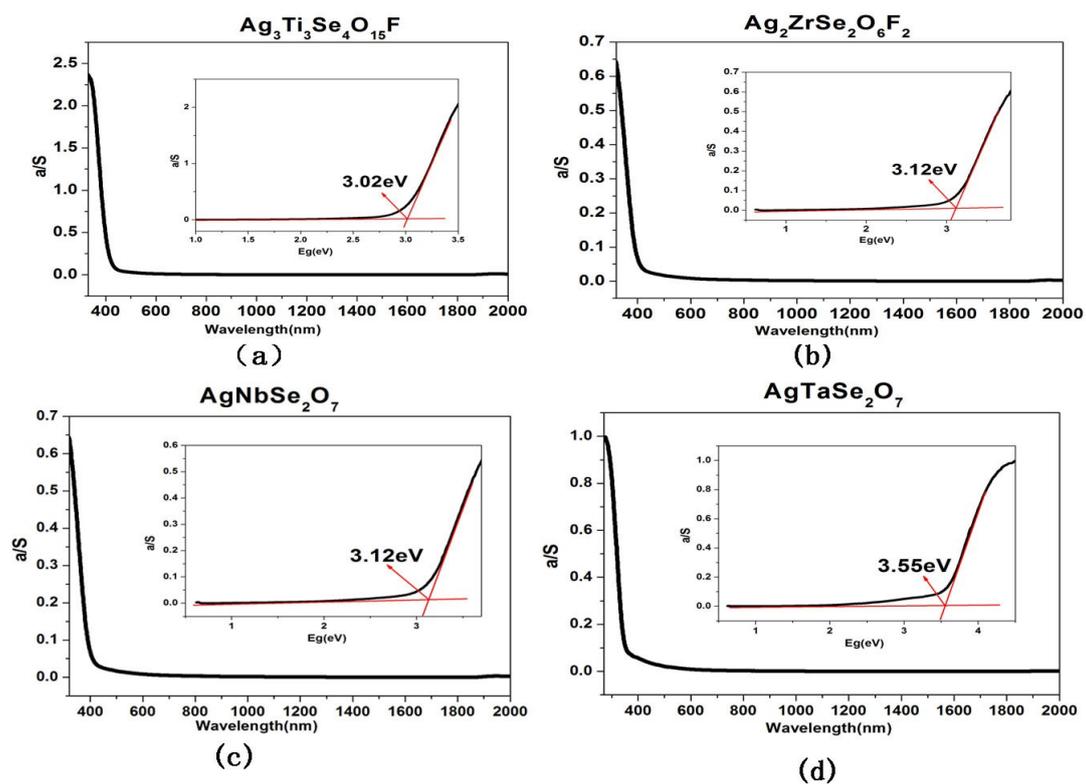


Fig S4. UV-Vis-NIR Diffuse Reflectance spectra of compounds **1(a)**, **2(b)**, **3(c)** and **4(d)**.