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Supporting Information

Computational Insights into Ternary Bimetallic Oxy-Chalcogenides

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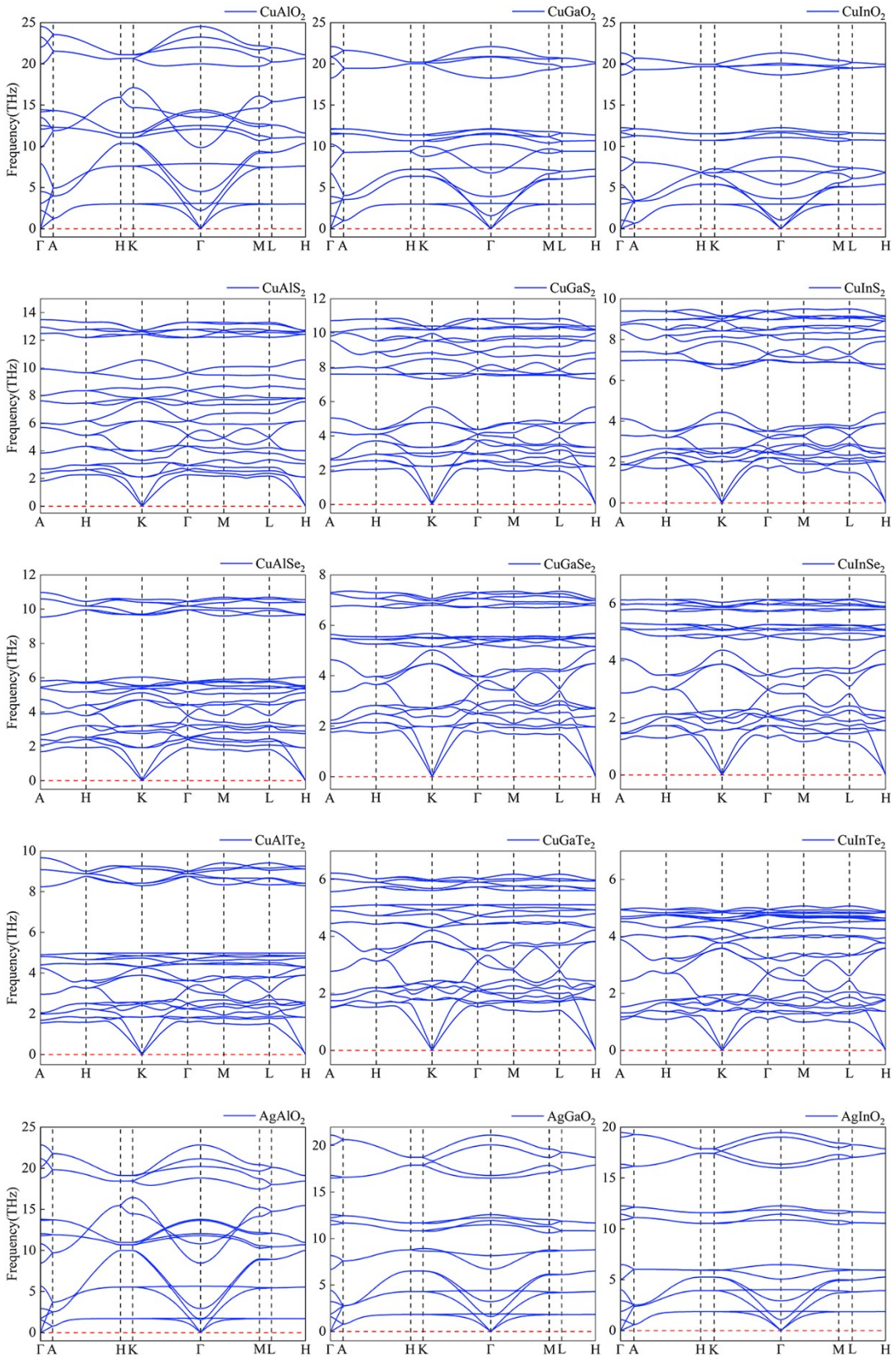
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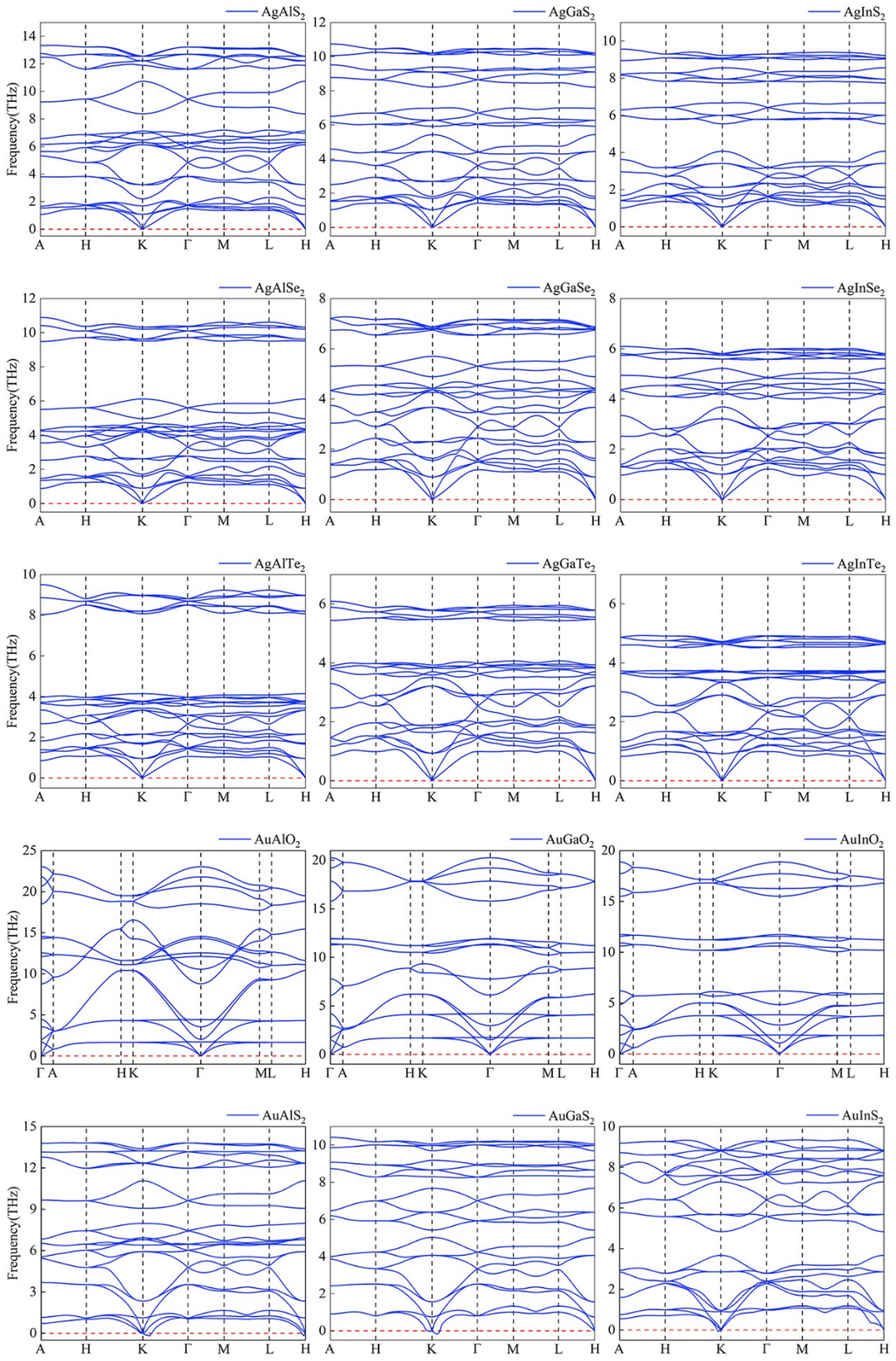
CuInO2
CuAlS2
CuGaS2
CuInS2
CuAlSe2
CuGaSe2
CuInSe2
CuAlTe2
CuGaTe2
CuInTe2
AgAlO2
AgGaO2
AgInO2
Frequency(THz)
Γ A H K Γ M L H
A H K Γ M L H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AuInS2
Frequency(THz)
A H K Γ M L H
Γ A H K Γ M L H

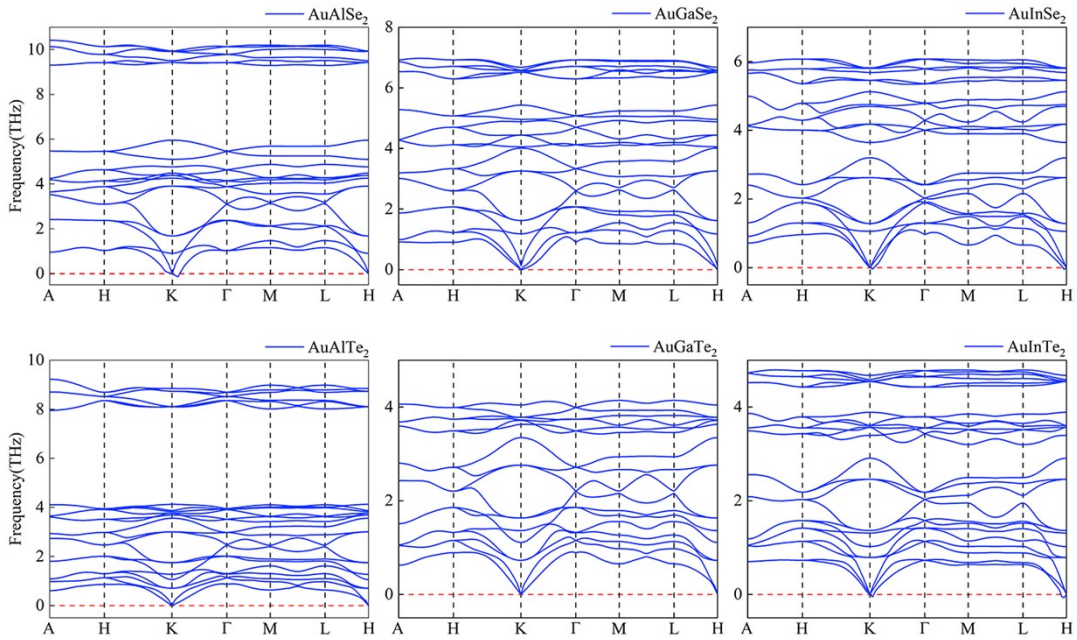
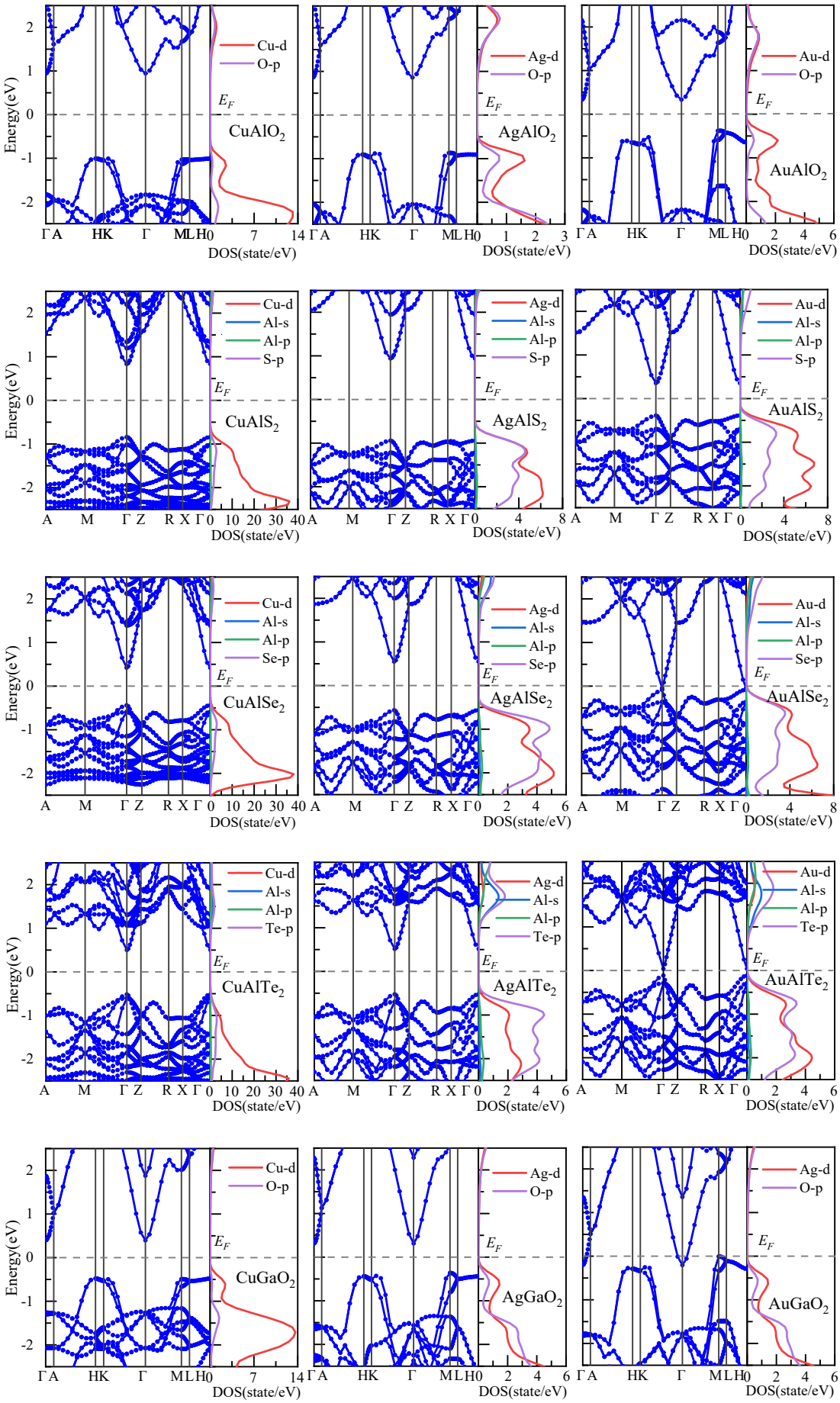
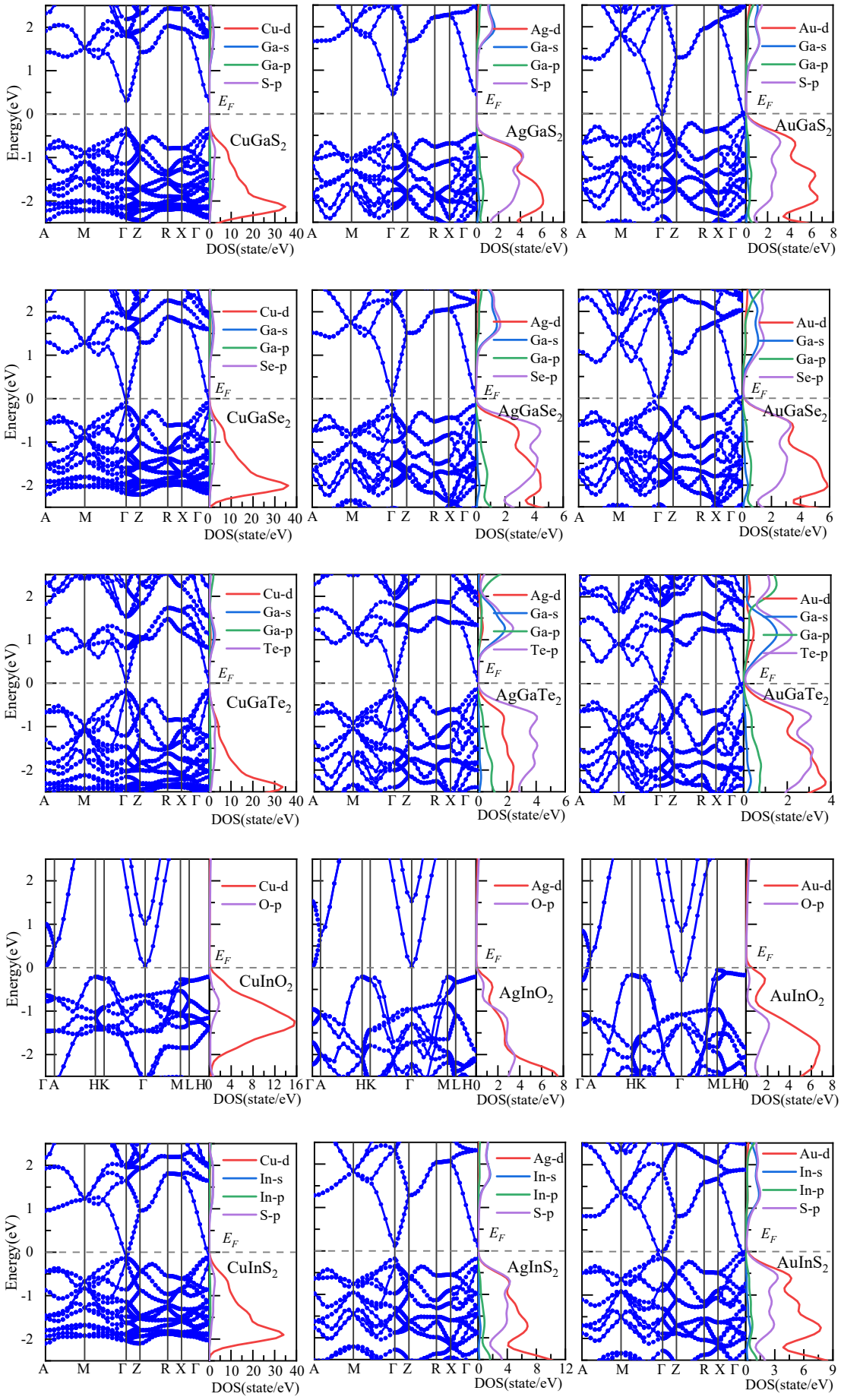


Figure S1. Phonon dispersion relations of M(IB)M'(IIIA)X_2 compounds.


Energy(eV)
DOS(state/eV)
Cu-d
O-p
Ag-d
Au-d
Al-s
Al-p
S-p
Se-p
Te-p
E_F
$CuAlO_2$
$AgAlO_2$
$AuAlO_2$
$CuAlS_2$
$AgAlS_2$
$AuAlS_2$
$CuAlSe_2$
$AgAlSe_2$
$AuAlSe_2$
$CuAlTe_2$
$AgAlTe_2$
$AuAlTe_2$
$CuGaO_2$
$AgGaO_2$
$AuGaO_2$
Γ A HK Γ ML H
A M Γ Z R X Γ


Energy(eV)
A M Γ Z R X Γ
DOS(state/eV)
Cu-d
Ga-s
Ga-p
S-p
E_F
$CuGaS_2$
Ag-d
Ga-s
Ga-p
S-p
E_F
$AgGaS_2$
Au-d
Ga-s
Ga-p
S-p
E_F
$AuGaS_2$
Cu-d
Ga-s
Ga-p
Se-p
E_F
$CuGaSe_2$
Ag-d
Ga-s
Ga-p
Se-p
E_F
$AgGaSe_2$
Au-d
Ga-s
Ga-p
Se-p
E_F
$AuGaSe_2$
Cu-d
Ga-s
Ga-p
Te-p
E_F
$CuGaTe_2$
Ag-d
Ga-s
Ga-p
Te-p
E_F
$AgGaTe_2$
Au-d
Ga-s
Ga-p
Te-p
E_F
$AuGaTe_2$
Γ A H K Γ M L H
Cu-d
O-p
E_F
$CuInO_2$
Ag-d
O-p
E_F
$AgInO_2$
Au-d
O-p
E_F
$AuInO_2$
Cu-d
In-s
In-p
S-p
E_F
$CuInS_2$
Ag-d
In-s
In-p
S-p
E_F
$AgInS_2$
Au-d
In-s
In-p
S-p
E_F
$AuInS_2$

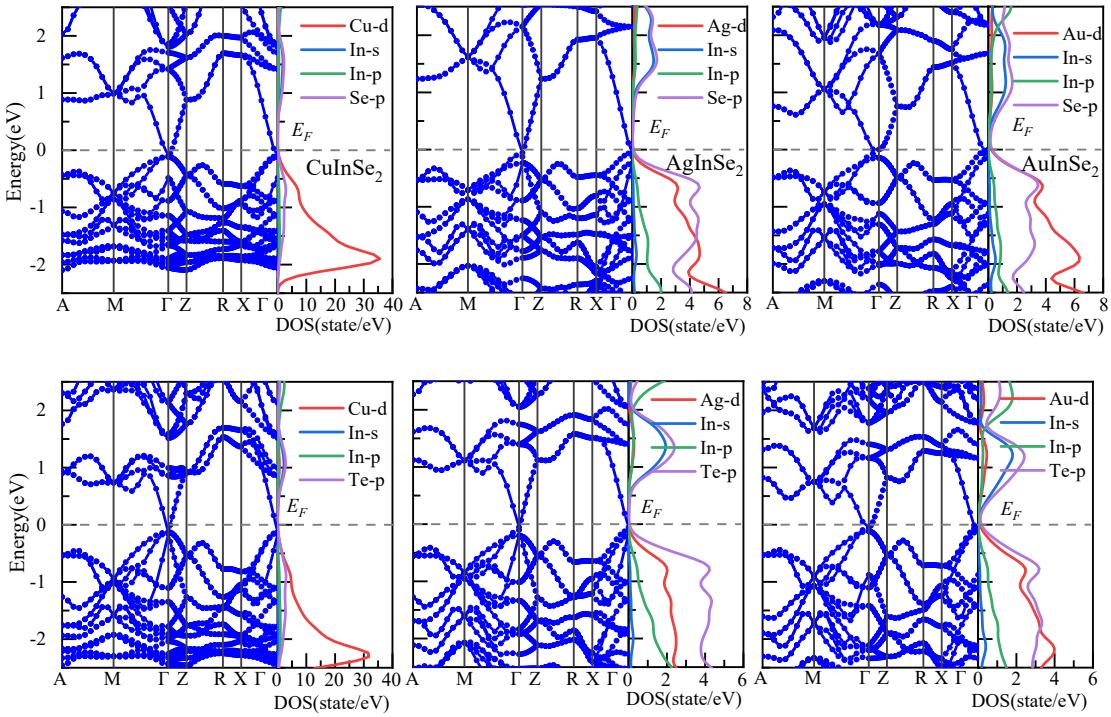


Figure S2. Band structures and density of states of M(IB)M'(IIIA)X_2 calculated using PBE functional.

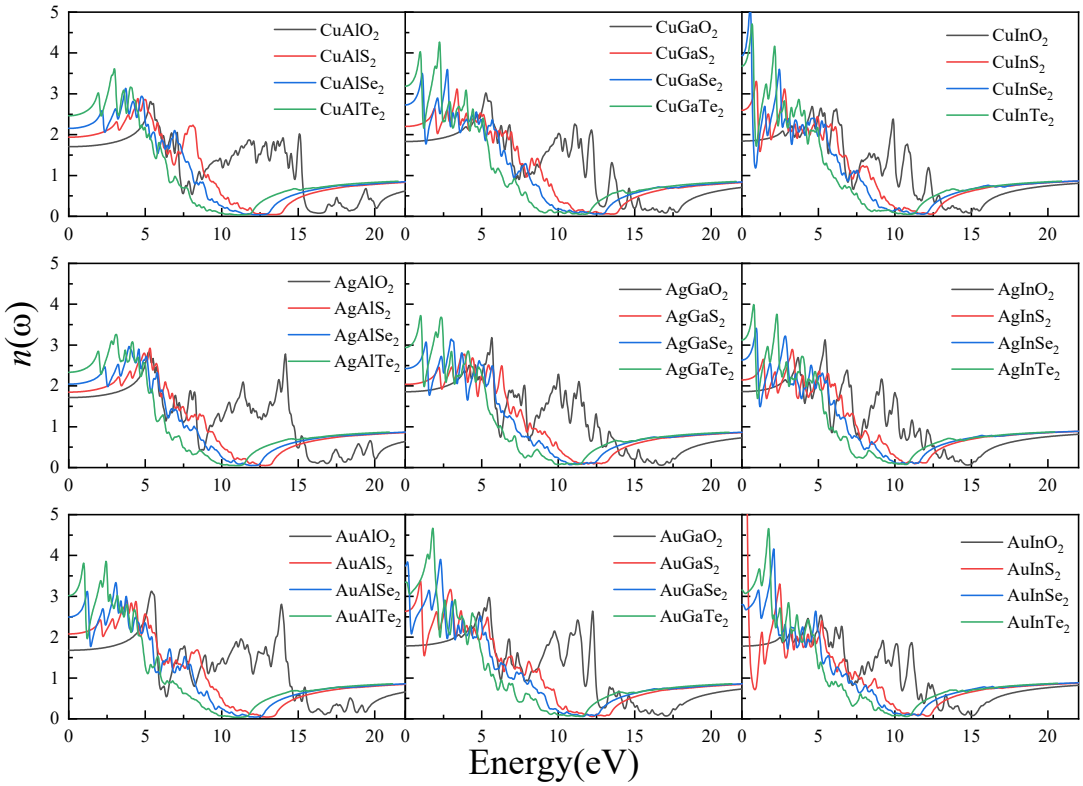


Figure S3. Refractive index $n(\omega)$ spectra of M(IB)M'(IIIA)X_2 in the range 0-22 eV calculated using HSE06 functional.

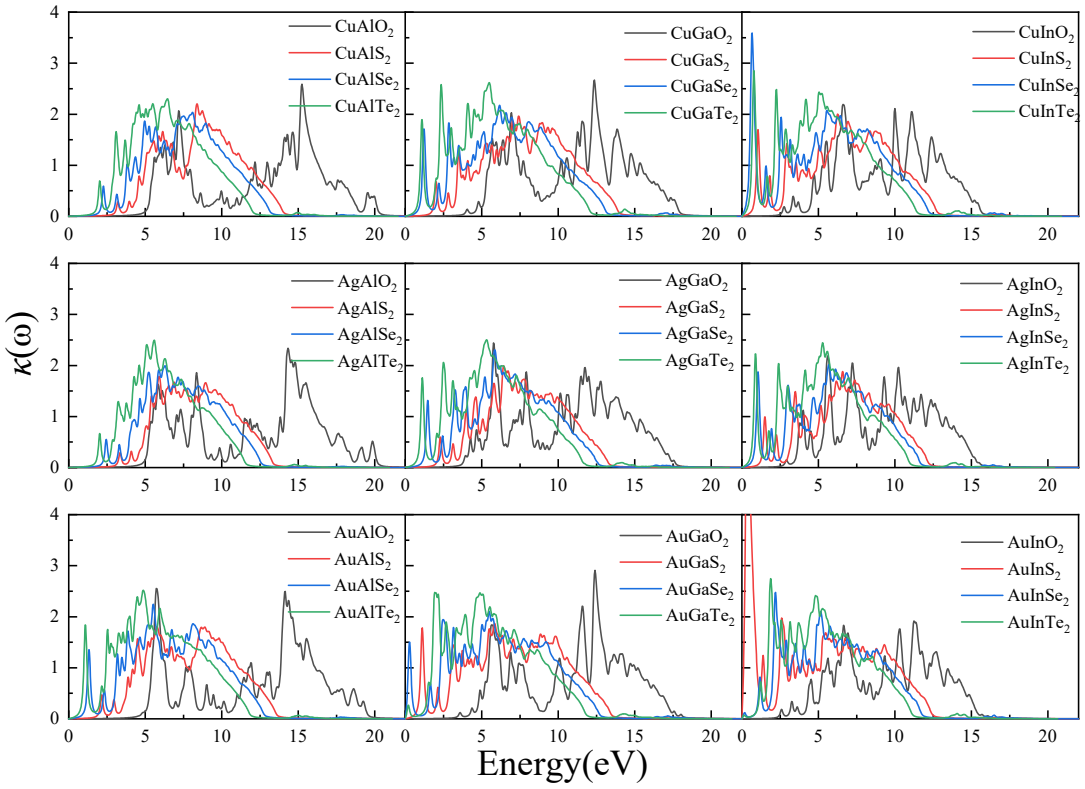


Figure S4. Extinction coefficient $\kappa(\omega)$ spectra of M(IB)M'(IIIA)X_2 in the range 0-22 eV calculated using HSE06 functional.

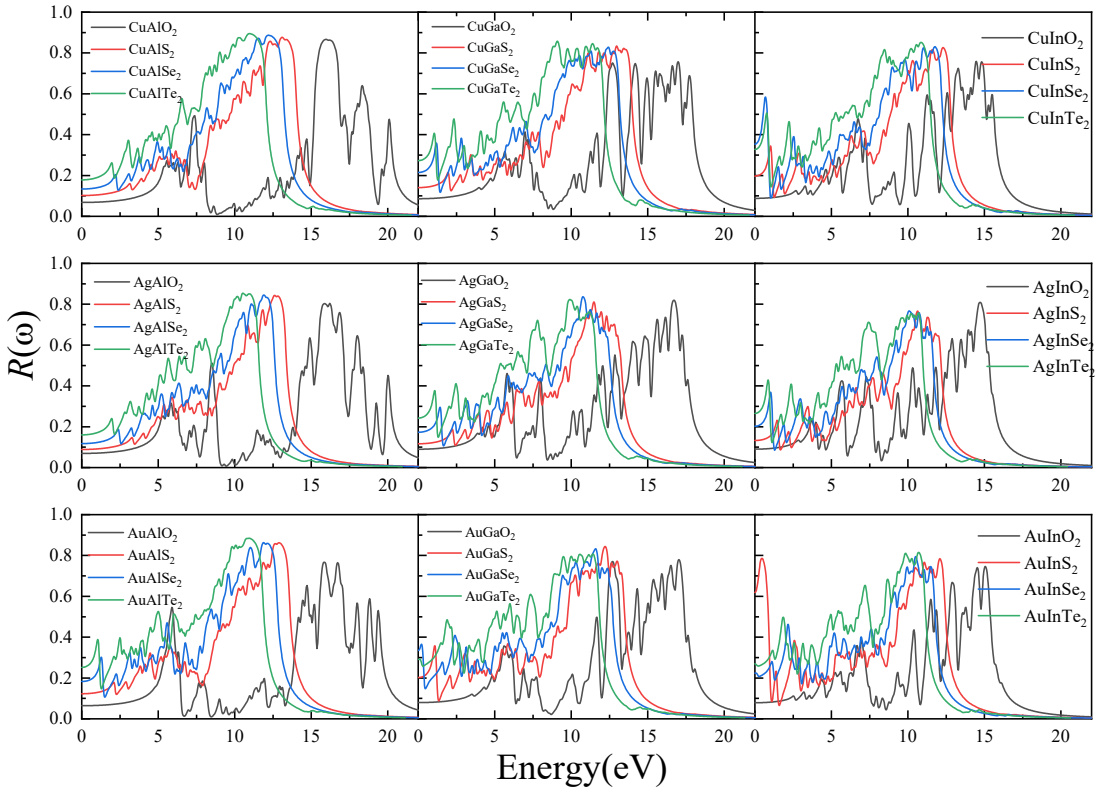


Figure S5. Reflectivity *R*(ω) spectra of M(IB)M'(IIIA)X_2 in the range 0-22 eV calculated using HSE06 functional.

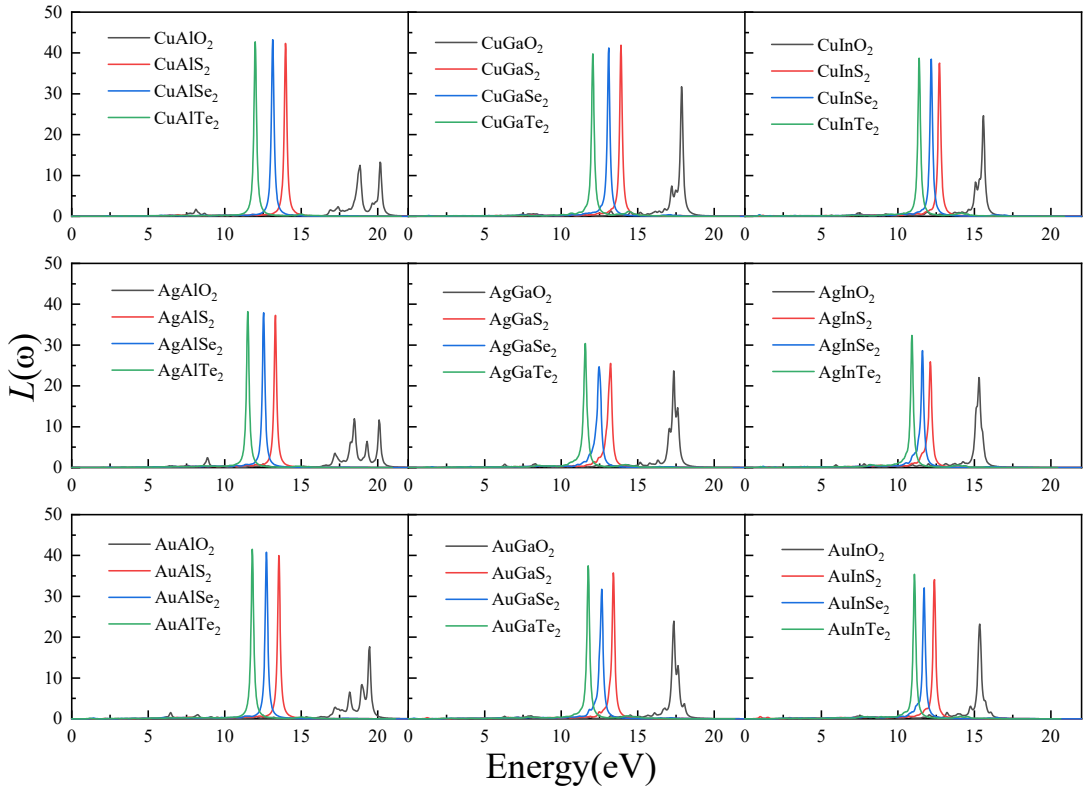


Figure S6. Energy-loss function $L(\omega)$ spectra of M(IB)M'(IIIA)X_2 in the range 0-22 eV calculated using HSE06 functional.

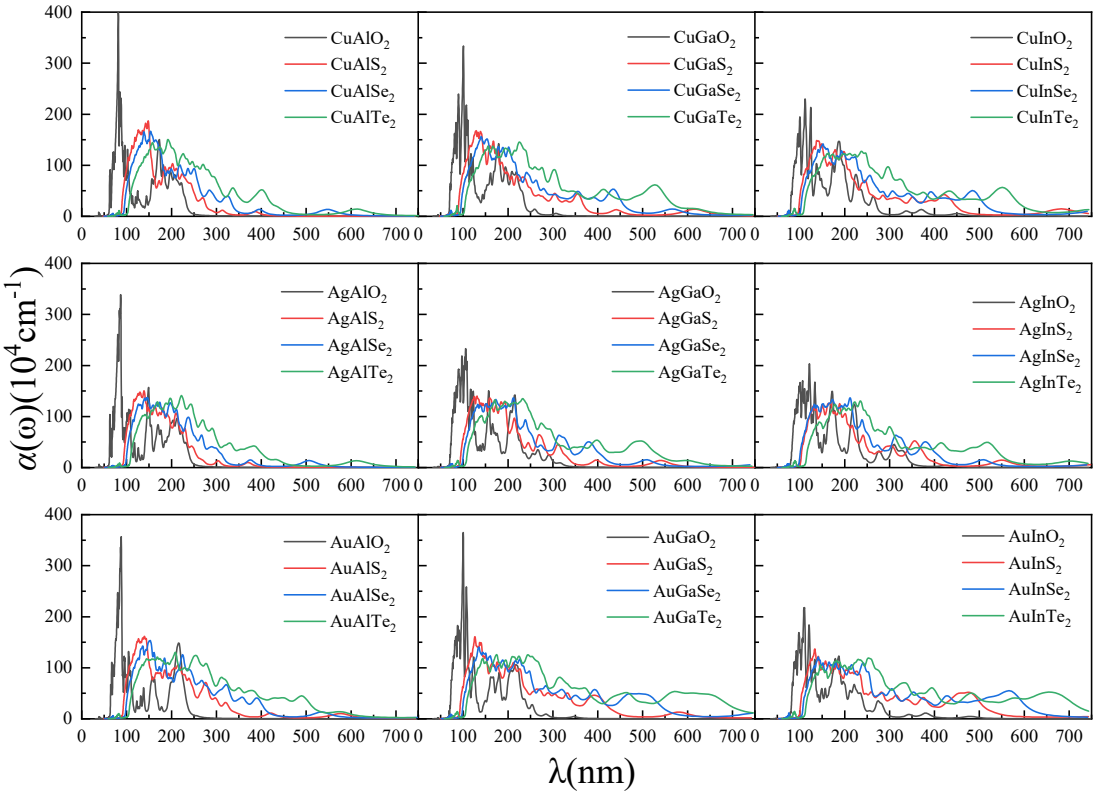


Figure S7. Absorption coefficient $\alpha(\omega)$ spectra of M(IB)M'(IIIA)X_2 in the range 0-750 nm calculated using HSE06 functional.

Sample	Lattice constant			Sample	Lattice constant			Sample	Lattice constant		
	a/Å	b/Å	c/Å		a/Å	b/Å	c/Å		a/Å	b/Å	c/Å
$CuAlO_2$	2.8409	2.4603	11.3300	$AgAlO_2$	2.8783	2.4926	12.0496	$AuAlO_2$	2.9019	2.5132	12.1392
$CuAlS_2$	5.3466	5.3466	10.5042	$AgAlS_2$	5.7521	5.7521	10.4438	$AuAlS_2$	5.6522	5.6522	10.6352
$CuAlSe_2$	5.6632	5.6632	11.0989	$AgAlSe_2$	6.0407	6.0407	11.0670	$AuAlSe_2$	5.9488	5.9488	11.2925
$CuAlTe_2$	6.1022	6.1022	12.0632	$AgAlTe_2$	6.4131	6.4131	12.2204	$AuAlTe_2$	6.3252	6.3252	12.3379
$CuGaO_2$	2.9917	2.5908	11.5022	$AgGaO_2$	3.0106	2.6072	12.3890	$AuGaO_2$	3.0200	2.6154	12.3314
$CuGaS_2$	5.3915	5.3915	10.6266	$AgGaS_2$	5.7761	5.7761	10.6432	$AuGaS_2$	5.7041	5.7041	10.7993
$CuGaSe_2$	5.6960	5.6960	11.2297	$AgGaSe_2$	6.0656	6.0656	11.2227	$AuGaSe_2$	5.9764	5.9864	11.4379
$CuGaTe_2$	6.1112	6.1112	12.1314	$AgGaTe_2$	6.4084	6.4084	12.2958	$AuGaTe_2$	6.3487	6.3487	12.3736
$CuInO_2$	3.3405	2.8905	11.6550	$AgInO_2$	3.3197	2.8749	12.6693	$AuInO_2$	3.3357	2.8889	12.5094
$CuInS_2$	5.6021	5.6021	11.2383	$AgInS_2$	5.9471	5.9471	11.5073	$AuInS_2$	5.8549	5.8549	11.6871
$CuInSe_2$	5.8937	5.8937	11.7847	$AgInSe_2$	6.2544	6.2544	11.9516	$AuInSe_2$	6.1419	6.1419	12.1851
$CuInTe_2$	6.3112	6.3112	12.5769	$AgInTe_2$	6.5855	6.5855	12.9397	$AuInTe_2$	6.5191	6.5191	12.9884

Table S1. Calculated lattice constants of the M(IB)M'(IIIA)X_2 compounds.

Note, for oxides, the lattice constants $\alpha=90^o$, $\beta=90^o$, $\gamma=120^o$

Table S2. Effective mass of charge carriers in the M(IB)M'(IIIA)X_2 compounds.

Compound	$m_n/m_p(m_0)$	Compound	$m_n/m_p(m_0)$	Compound	$m_n/m_p(m_0)$	Compound	$m_n/m_p(m_0)$
$CuAlO_2$	0.15 0.26	$CuAlS_2$	0.01 0.02	$CuAlSe_2$	0.01 0.01	$CuAlTe_2$	/ 0.01
$CuGaO_2$	0.06 0.17	$CuGaS_2$	0.01 0.01	$CuGaSe_2$	/ 0.01	$CuGaTe_2$	/ 0.01
$CuInO_2$	0.04 0.13	$CuInS_2$	0.01 0.03	$CuInSe_2$	/ 0.03	$CuInTe_2$	/ 0.02
$CuAlO_2$	0.14 0.26	$AgAlS_2$	0.01 0.02	$AgAlSe_2$	/ 0.01	$AgAlTe_2$	/ 0.01
$CuGaO_2$	0.06 0.20	$AgGaS_2$	0.01 0.01	$AgGaSe_2$	/ 0.01	$AgGaTe_2$	/ /
$CuInO_2$	0.04 0.11	$AgInS_2$	/ 0.01	$AgInSe_2$	/ 0.01	$AgInTe_2$	/ /
$AgAlO_2$	0.15 0.20	$AuAlS_2$	0.01 0.02	$AuAlSe_2$	/ 0.01	$AuAlTe_2$	/ /
$AgGaO_2$	0.07 0.13	$AuGaS_2$	/ 0.01	$AuGaSe_2$	/ /	$AuGaTe_2$	/ /
$AgInO_2$	0.04 0.11	$AuInS_2$	/ 0.01	$AuInSe_2$	/ 0.01	$AuInTe_2$	/ 0.01

m_0=9.10938215 × 10^{-31} kg

Table S3. Bader charge states of each element in the M(IB)M'(IIIA)X_2 compounds.

Compound	charge state (e)		
	M	M'	X
$CuAlO_2$	+0.64	+3.00	−1.82
$CuAlS_2$	+0.54	+3.00	−1.77
$CuAlSe_2$	+0.36	+3.00	−1.68
$CuAlTe_2$	+0.15	+3.00	−1.58
$CuGaO_2$	+0.61	+3.00	−1.81
$CuGaS_2$	+0.49	+3.00	−1.75
$CuGaSe_2$	+0.36	+3.00	−1.68
$CuGaTe_2$	+0.14	+3.00	−1.57
$CuInO_2$	+0.48	+3.00	−1.74
$CuInS_2$	+0.49	+2.91	−1.70
$CuInSe_2$	+0.36	+2.92	−1.64
$CuInTe_2$	+0.13	+3.00	−1.57
$AgAlO_2$	+0.55	+3.00	−1.77
$AgAlS_2$	+0.42	+3.00	−1.71
$AgAlSe_2$	+0.31	+3.00	−1.66
$AgAlTe_2$	+0.13	+3.00	−1.56
$AgGaO_2$	+0.46	+3.00	−1.73
$AgGaS_2$	+0.42	+3.00	−1.71
$AgGaSe_2$	+0.31	+3.00	−1.65
$AgGaTe_2$	+0.10	+3.00	−1.55
$AgInO_2$	+0.58	+3.00	−1.79
$AgInS_2$	+0.39	+2.95	−1.67
$AgInSe_2$	+0.31	+2.95	−1.63
$AgInTe_2$	+0.08	+2.98	−1.53
$AuAlO_2$	+0.47	+3.00	−1.74
$AuAlS_2$	+0.21	+3.00	−1.60
$AuAlSe_2$	+0.05	+3.00	−1.52
$AuAlTe_2$	−0.25	+3.00	−1.37
$AuGaO_2$	+0.48	+3.00	−1.74
$AuGaS_2$	+0.21	+3.00	−1.60
$AuGaSe_2$	+0.04	+3.00	−1.52
$AuGaTe_2$	−0.30	+3.00	−1.35
$AuInO_2$	+0.46	+3.00	−1.73
$AuInS_2$	+0.20	+2.94	−1.57
$AuInSe_2$	−0.04	+2.94	−1.45
$AuInTe_2$	−0.31	+2.98	−1.33