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Machine Learning and Density Functional Theory Simulation of Electronic Structural Properties for Novel Quaternary Semiconductors

Mengwei Gao[1], Bo Cai[1,2*], Gaoyu Liu[1], Lili Xu[1], Shengli Zhang[1*] and Haibo Zeng[1*]

1. MIIT Key Laboratory of Advanced Display Materials and Devices, School of Materials Science and Engineering, Nanjing University of Science and Technology, Nanjing 210094, China. E-mail: zhangslvip@njust.edu.cn; zeng.haibo@njust.edu.cn

2. State Key Laboratory of Organic Electronics and Information Displays & Institute of Advanced Materials (IAM), Nanjing University of Posts & Telecommunications, 9 Wenyuan Road, Nanjing 210023, China. E-mail: iambcai@njupt.edu.cn

CONTENT

Supplementary Tables

Table S1. Elemental properties used to compute elemental-property-based attributes. Elemental property is taken from that dataset available with the Wolfram programming language, unless otherwise specified.

Atomic Number mean/maxdiff/dev/ max/min/most	Mendeleev Number mean/maxdiff/dev/ max/min/most	Atomic Weight mean/maxdiff/dev/ max/min/most	Melting Temperature mean/maxdiff/dev/ max/min/most
Column mean/maxdiff/dev/ max/min/most	Row mean/maxdiff/dev/ max/min/most	Covalent Radius mean/maxdiff/dev/ max/min/most	Electronegativity mean/maxdiff/dev/ max/min/most
s Valence Electrons mean/maxdiff/dev/ max/min/most	p Valence Electrons mean/maxdiff/dev/ max/min/most	d Valence Electrons mean/maxdiff/dev/ max/min/most	f Valence Electrons mean/maxdiff/dev/ max/min/most
Total Valence Electrons mean/maxdiff/dev/ max/min/most	Unfilled s states mean/maxdiff/dev/ max/min/most	Unfilled p states mean/maxdiff/dev/ max/min/most	Unfilled d states mean/maxdiff/dev/ max/min/most
Unfilled f states mean/maxdiff/dev/ max/min/most	Total Unfilled states mean/maxdiff/dev/ max/min/most	Specific Volume of 0 K Ground state mean/maxdiff/dev/ max/min/most	Bandap Energy of 0 K Ground state mean/maxdiff/dev/ max/min/most
Frac s/p/d/f Valence	Ionic Char mean/max	Magnetic Moment (per atom) of 0 K Ground state mean/maxdiff/dev/	Space Group Number of 0 K Group state mean/maxdiff/dev/

		max/min/most	max/min/most

Table S2. In 2180 quaternary semiconductors, the materials whose bandgap values in the range of 1.6 ~ 3.2 eV, which are predicted by the ML training model.

Na_2AuGaS_4	$Li_2PdHfTe_4$	Fe_2LiAuS_4	Co_2LiInS_4
$Li_2PdHfSe_4$	$Li_2PtCrSe_4$	$Na_2AgMoTe_4$	Fe_2KInSe_4
$K_2PdSiSe_4$	$Na_2PtCrSe_4$	Fe_2PdZnS_4	Mg_2LiAlO_4
$K_2FeSiSe_4$	$K_2NaMoTe_4$	$Na_2MgCrTe_4$	$K_2PtSnTe_4$
$Na_2PdHfSe_4$	Ni_2MgPdO_4	Mg_2CoZnS_4	$K_2AuGaTe_4$
K_2AuGaS_4	Ni_2AgAlO_4	$Ag_2MgCrSe_4$	Ag_2ZnSiO_4
K_2PtGeS_4	Ag_2MgSiO_4	Pd_2LiGaO_4	$Na_2AuAlTe_4$
$Na_2MgSiSe_4$	$K_2AuGaSe_4$	$K_2GaInTe_4$	$Na_2PtSiTe_4$
Li_2PtCrS_4	Ag_2MgZrO_4	Ag_2FeZrS_4	Ni_2CoZnO_4
$Na_2MgZrSe_4$	$Na_2ZnSnSe_4$	$Na_2PdZrTe_4$	Co_2KAlS_4
$Na_2ZnHfSe_4$	Ag_2NaMoO_4	Ni_2MgFeO_4	Zn_2FeCoO_4
$Li_2MgZrSe_4$	$Li_2ZnHfTe_4$	Co_2MgNiO_4	Fe_2KAlS_4
$K_2AlInSe_4$	$Ag_2NaCrSe_4$	$Li_2PtHfTe_4$	Zn_2LiAlS_4
K_2PtCrS_4	Co_2NaAuS_4	$K_2PdSnTe_4$	$Li_2PdGeTe_4$
Li_2PtHfS_4	$K_2MgSiTe_4$	$Na_2NiGeTe_4$	$Li_2FeGeTe_4$
$K_2MgCrSe_4$	Co_2KAuS_4	$Na_2CoGeTe_4$	Zn_2FeNiO_4
$K_2MgTiSe_4$	Co_2AgAlO_4	$K_2FeZrTe_4$	Fe_2CoZnO_4
Li_2AuInO_4	Ag_2MgTiO_4	Pd_2KAlO_4	$Mg_2LiAlSe_4$
Li_2PtSnO_4	Co_2MgPdO_4	Ni_2CoPdS_4	$K_2AuAlTe_4$
$Na_2ZnSiSe_4$	$K_2PtGeSe_4$	Ni_2MgCoO_4	$Na_2MgSnTe_4$
$Li_2MgSiSe_4$	Ag_2MgCO_4	Ag_2FeGeO_4	Ni_2NaAlS_4
$K_2ZnHfSe_4$	Na_2GaSbS_4	$Co_2MgPdSe_4$	Co_2LiInO_4
K_2AuSbO_4	Ag_2PdHfO_4	$Ag_2MgTiSe_4$	Zn_2MgCoO_4
Li_2AuSbO_4	Ag_2NaNbO_4	$K_2PdGeTe_4$	Zn_2CoNiO_4
$K_2NiHfSe_4$	Li_2KMoTe_4	Ag_2ZnZrS_4	Co_2LiGaS_4
$K_2CoHfSe_4$	$Na_2LiMoTe_4$	Mg_2NiZnS_4	$Fe_2LiAuTe_4$

$K_2MgSnSe_4$	Ag_2KNbSe_4	Fe_2CoPdS_4	Zn_2MgNiO_4
$Na_2NiSiSe_4$	$Ag_2MgHfSe_4$	Mg_2FeZnS_4	$Zn_2AgAlSe_4$
$K_2NaCrSe_4$	Zn_2AgAlS_4	$Pd_2MgFeSe_4$	Mg_2NaGaS_4
$K_2FeHfSe_4$	Ag_2MgCS_4	$Na_2ZnCrTe_4$	$Li_2MgSiTe_4$
$Li_2ZnSiSe_4$	Ag_2MgTiS_4	$Na_2FeGeTe_4$	Mg_2NaAlS_4
$Li_2NaCrSe_4$	Mg_2AgGaS_4	Pd_2LiAlS_4	$Li_2CoTiTe_4$
K_2PtSnS_4	$Li_2PtTiSe_4$	$Na_2PdCrTe_4$	$Li_2ZnCrTe_4$
K_2AuInS_4	Zn_2AgAlO_4	Fe_2KAuO_4	$Co_2LiInSe_4$
$K_2PdHfSe_4$	$K_2PdSiTe_4$	$K_2PtTiSe_4$	$Li_2NiGeTe_4$
$Na_2AlGaSe_4$	$Ag_2NaNbSe_4$	Ag_2PdGeS_4	Ni_2LiInS_4
$Li_2NiZrSe_4$	Zn_2MgPdS_4	Ag_2PdCS_4	Ni_2LiGaS_4
$Li_2AlGaSe_4$	Ag_2PdCO_4	$Na_2MgSiTe_4$	$K_2PtZrTe_4$
Na_2KCrSe_4	Co_2AgAlS_4	$Co_2AgAlSe_4$	Ag_2ZnGeS_4
$Li_2FeZrSe_4$	$K_2LiCrTe_4$	$Na_2PdSnTe_4$	Ni_2KAlS_4
$K_2ZnGeSe_4$	$K_2PtCrSe_4$	$Na_2PdTiTe_4$	Co_2NiZnO_4
$Li_2CoZrSe_4$	Ag_2NiHfO_4	Ni_2LiAuO_4	Fe_2NiZnO_4
Li_2AuInS_4	Ag_2KCrO_4	Fe_2LiAuO_4	Co_2NaAlS_4
$Na_2MgGeSe_4$	Fe_2MgPdO_4	$Na_2NiCrTe_4$	Fe_2KGaS_4
$K_2NiGeSe_4$	Ag_2KMoSe_4	Ag_2FeCrS_4	Co_2FeZnO_4
$K_2LiCrSe_4$	Ni_2FePdO_4	Ag_2CoGeO_4	$Co_2NaAuSe_4$
Na_2GaSbO_4	Fe_2MgPdS_4	Ag_2NiCrS_4	$Li_2NiTiTe_4$
$Li_2MgGeSe_4$	Co_2NiPdO_4	$Pd_2MgCoSe_4$	$Li_2CoGeTe_4$
Li_2PtSnS_4	$Li_2PtZrSe_4$	Pd_2KAlSe_4	$K_2AuSbTe_4$
Na_2PtHfS_4	Ag_2LiMoO_4	$K_2CoTiTe_4$	Co_2KAlO_4
$Na_2PdSiSe_4$	Ni_2AgAlS_4	Fe_2NaAuO_4	$Li_2PdSnTe_4$
Li_2ZnCSe_4	$K_2AlGaTe_4$	$Na_2AgCrTe_4$	$Ag_2MgGeSe_4$
Na_2PtSnS_4	Fe_2AgAlS_4	$Na_2CoCrTe_4$	$K_2AlSbTe_4$
Li_2PtZrS_4	Na_2KCrTe_4	Fe_2NaInS_4	Ni_2FeZnO_4
Na_2AuInS_4	Ni_2MgPdS_4	$Pd_2MgNiSe_4$	$Li_2FeTiTe_4$

$Li_2PdTiSe_4$	Fe_2NiPdO_4	$Na_2FeTiTe_4$	Ag_2AlGaO_4
$Li_2PdSiSe_4$	Ag_2LiNbS_4	Zn_2MgNiS_4	$Li_2ZnGeTe_4$
Li_2PdCSe_4	$K_2NiSiTe_4$	Ag_2NiGeO_4	Co_2KAuSe_4
$Na_2CoSiSe_4$	Co_2MgPdS_4	$Na_2CoTiTe_4$	$Li_2FeCrTe_4$
$Li_2PdCrSe_4$	Ag_2NaCrO_4	Zn_2MgCoS_4	$Ag_2AlGaSe_4$
$Na_2FeZrSe_4$	$K_2CoSiTe_4$	$K_2AgCrTe_4$	$Ag_2PdZrSe_4$
$Li_2AgCrSe_4$	Mg_2AgAlS_4	$Na_2FeCrTe_4$	$Na_2AuGaTe_4$
Li_2CoCSe_4	Mg_2FePdS_4	$K_2PdCrTe_4$	$K_2PtGeTe_4$
Li_2AuSbS_4	Fe_2CoPdO_4	$Fe_2MgPdSe_4$	Co_2NaGaS_4
$K_2CoCrSe_4$	Ag_2LiCrS_4	Ag_2CoCrS_4	Fe_2NaAlS_4
K_2ZnCSe_4	$K_2FeSiTe_4$	$K_2NiSnTe_4$	$Ag_2PdCrSe_4$
$Na_2CoZrSe_4$	Mg_2PdZnS_4	$K_2FeCrTe_4$	$Na_2PtGeTe_4$
$Na_2AlInSe_4$	Ag_2CoHfO_4	$Na_2PdGeTe_4$	Ni_2NaGaS_4
K_2AuSbS_4	Mg_2CoPdS_4	Fe_2CoNiS_4	$Ag_2ZnSiSe_4$
$K_2FeZrSe_4$	Co_2LiAuS_4	$K_2FeTiTe_4$	Zn_2LiAlO_4
$Na_2MgCrSe_4$	Mg_2NiPdS_4	$K_2CoCrTe_4$	Mg_2LiGaO_4
Li_2NiCSe_4	Co_2FePdO_4	Pd_2FeNiS_4	$Li_2CoCrTe_4$
Li_2FeCSe_4	Pd_2MgNiS_4	$K_2CoSnTe_4$	Pd_2AgInS_4
$Li_2AlInSe_4$	$Li_2AuSbSe_4$	$Ag_2FeSiSe_4$	Li_2PdCTe_4
$Na_2NiZrSe_4$	$K_2NaNbTe_4$	$K_2NiGeTe_4$	Mg_2KGaSe_4
$Na_2FeSiSe_4$	$Ag_2LiMoSe_4$	$K_2CoGeTe_4$	Co_2KGaS_4
$K_2ZnZrSe_4$	Pd_2MgZnS_4	$K_2NiCrTe_4$	Ni_2NaAlO_4
$K_2PdSnSe_4$	Fe_2PdZnO_4	Li_2PtCTe_4	$Li_2NiCrTe_4$
$Li_2MgCrSe_4$	Ni_2PdZnO_4	$K_2FeGeTe_4$	Ni_2KAuO_4
$Li_2NiSiSe_4$	Ag_2LiNbO_4	$Pd_2NaAlSe_4$	Ni_2KGaS_4
$Li_2AgNbSe_4$	$K_2MgCrTe_4$	$Na_2NiTiTe_4$	$Ag_2CoZrSe_4$
$K_2MgHfTe_4$	Ag_2NiSiS_4	$K_2FeSnTe_4$	$Na_2PtZrTe_4$
$Li_2CoSiSe_4$	Pd_2AgAlO_4	Ni_2MgZnS_4	Li_2ZnCTe_4
Li_2KCrSe_4	Ag_2FeCrO_4	Pd_2FeCoS_4	$Na_2GaInTe_4$

$Na_2LiCrSe_4$	Pd_2AgAlS_4	Zn_2MgFeS_4	$Ag_2NiZrSe_4$
$K_2PdGeSe_4$	Ni_2CoPdO_4	Ag_2PdCrO_4	Ni_2LiGaO_4
$K_2NiZrSe_4$	Fe_2KAuSe_4	Co_2FeNiS_4	K_2MgCTe_4
$Li_2FeSiSe_4$	Ag_2CoSiS_4	$K_2NiTiTe_4$	Mg_2LiGaS_4
$K_2CoZrSe_4$	Zn_2FePdO_4	Mg_2FeZnO_4	$Fe_2MgCoTe_4$
$K_2NiCrSe_4$	Zn_2NiPdO_4	Ag_2NiTiS_4	$Fe_2LiInSe_4$
$Li_2PdZrSe_4$	Fe_2AgAlO_4	$K_2ZnCrTe_4$	Ag_2KCrTe_4
$Li_2AgMoSe_4$	Zn_2CoPdO_4	$Li_2AuAlTe_4$	$Ag_2FeZrSe_4$
$Na_2NiGeSe_4$	Co_2AgGaO_4	Mg_2CoZnO_4	Mg_2KAlO_4
$Na_2CoCrSe_4$	Ni_2AgGaO_4	$Li_2PtSiTe_4$	$K_2PtCrTe_4$
Na_2PdCSe_4	Pd_2MgCoS_4	$Li_2PtZrTe_4$	$Li_2MgCrTe_4$
$K_2GaInSe_4$	Ag_2PdSiS_4	Mg_2NiZnO_4	$Li_2AlSbTe_4$
$K_2PdCrSe_4$	Fe_2AgGaO_4	$K_2PdTiTe_4$	Mg_2NaAlO_4
K_2PdCSe_4	Fe_2KAuS_4	$Na_2CoSnTe_4$	$Ag_2ZnZrSe_4$
$K_2NiSnSe_4$	Co_2PdZnO_4	Ag_2CoTiS_4	Fe_2MgPtS_4
Na_2ZnCSe_4	Na_2InSbS_4	$Na_2NiSnTe_4$	$Li_2MgTiTe_4$
$Li_2PdGeSe_4$	$K_2AlInTe_4$	Ag_2FeTiS_4	Ni_2KAlO_4
$K_2CoGeSe_4$	Ag_2FeHfO_4	Ni_2FeCoS_4	$Co_2NaAlSe_4$
K_2PtHfS_4	Ag_2MgCrS_4	Ag_2NiZrO_4	Pd_2KGaSe_4
$K_2AgMoSe_4$	$K_2MgGeTe_4$	Fe_2AgGaS_4	Fe_2AgInS_4
K_2NiCSe_4	$Fe_2NaAuSe_4$	Fe_2MgZnS_4	$Fe_2MgCoSe_4$
K_2MgCSe_4	Ag_2PdSiO_4	$Na_2ZnSiTe_4$	Co_2KAlSe_4
$Na_2PdTiSe_4$	$K_2AuSbSe_4$	Pd_2CoNiS_4	Pd_2NaInS_4
$Na_2AgMoSe_4$	$Ag_2LiNbSe_4$	Zn_2AgGaO_4	$K_2PtTiTe_4$
$Na_2PdCrSe_4$	Ag_2NiTiO_4	$Ag_2CoSiSe_4$	$Fe_2MgNiSe_4$
Na_2PtZrS_4	$Na_2PtZrSe_4$	Co_2MgZnS_4	$Ag_2PdTiSe_4$
$Na_2AgNbSe_4$	Mg_2NiPdO_4	Co_2PdZnS_4	$Ag_2FeHfTe_4$
Na_2NiCSe_4	Ag_2CoCrO_4	Co_2LiAlO_4	Zn_2AgInS_4
Na_2AuSbS_4	Pd_2FeCoO_4	Co_2AgGaS_4	$Zn_2NaAlSe_4$

$K_2FeGeSe_4$	Mg_2PdZnO_4	Ni_2PdZnS_4	Co_2KAlTe_4
$Na_2MgHfTe_4$	K_2InSbS_4	Co_2KInS_4	$Fe_2NaAuTe_4$
$Na_2AgCrSe_4$	Ag_2MgGeS_4	Ag_2ZnCO_4	Mg_2KInSe_4
$Na_2PdZrSe_4$	Mg_2FePdO_4	Zn_2FePdS_4	$Li_2GaInTe_4$
$K_2AgNbSe_4$	Mg_2CoPdO_4	$Li_2PtSnTe_4$	$Co_2LiAlSe_4$
$Li_2ZnGeSe_4$	$Ag_2MgZrSe_4$	$Li_2AuInTe_4$	Co_2AgInS_4
$Li_2NiGeSe_4$	Ag_2FeTiO_4	Ag_2KMoTe_4	$K_2InSbTe_4$
$Li_2ZnZrSe_4$	$Ag_2LiCrSe_4$	Ag_2CoZrO_4	$Fe_2LiAlSe_4$
$K_2FeCrSe_4$	Ag_2CoTiO_4	$K_2ZnSnTe_4$	Mg_2KAlSe_4
$K_2PdZrSe_4$	$Na_2MgZrTe_4$	Ag_2ZnTiO_4	$Ni_2LiAlSe_4$
$Na_2PdGeSe_4$	Pd_2MgFeS_4	Ni_2AgGaS_4	Pd_2KGaS_4
Li_2PtTiS_4	Ag_2FeSiS_4	Zn_2CoPdS_4	$Na_2PtCrTe_4$
Na_2AuSbO_4	Ag_2AlGaS_4	$Ni_2MgPdSe_4$	$Li_2FeSiTe_4$
$Li_2FeGeSe_4$	Ag_2ZnSiS_4	$Ag_2NiSiSe_4$	Ni_2LiInO_4
$Li_2CoCrSe_4$	$Li_2NaMoTe_4$	$Li_2PtCrTe_4$	Ag_2MgSnS_4
$K_2FeTiSe_4$	$Li_2AlSbSe_4$	Zn_2NiPdS_4	$Pd_2FeCoSe_4$
$Li_2CoGeSe_4$	Ag_2LiCrO_4	$Li_2PtGeTe_4$	Ag_2PtCrS_4
$Li_2ZnCrSe_4$	Mg_2AgAlO_4	$Na_2FeSnTe_4$	$K_2GaSbTe_4$
K_2CoCSe_4	$Na_2InSbSe_4$	Ag_2FeZrO_4	$Na_2PtTiTe_4$
$K_2NiTiSe_4$	$Li_2InSbSe_4$	Zn_2KAlS_4	$Zn_2LiAlSe_4$
$Li_2FeCrSe_4$	Mg_2AgGaO_4	Ag_2ZnCrS_4	$Mg_2NaGaSe_4$
$Na_2ZnZrSe_4$	$Fe_2LiAuSe_4$	Ni_2FeCoO_4	$Ag_2CoCrSe_4$
$K_2CoTiSe_4$	Ag_2ZnHfS_4	$Li_2AuGaTe_4$	Pd_2LiInO_4
$Na_2ZnGeSe_4$	Ag_2FeCS_4	$K_2PtHfTe_4$	$Pt_2LiAuSe_4$
$K_2ZnCrSe_4$	$Li_2NaCrTe_4$	Ag_2MgGeO_4	$Co_2MgFeSe_4$
Na_2CoCSe_4	Mg_2CoNiS_4	Ag_2ZnTiS_4	Ni_2AgInS_4
$Li_2NiCrSe_4$	$Na_2PtTiSe_4$	Co_2LiGaO_4	$Mg_2LiGaSe_4$
Na_2FeCSe_4	Fe_2NaInO_4	Ni_2NaAuO_4	$Ag_2ZnCrSe_4$
Li_2PtCSe_4	Ag_2NiHfS_4	$Ni_2AgAlSe_4$	$Fe_2MgZnSe_4$

$Na_2CoGeSe_4$	Ag_2PdHfS_4	Fe_2CoNiO_4	Zn_2KInS_4
$Na_2FeHfTe_4$	$Na_2AlSbSe_4$	Ag_2AlInS_4	$Ag_2FeCrSe_4$
$Na_2NiHfTe_4$	$Na_2GaSbSe_4$	$Li_2PtTiTe_4$	$Pd_2FeNiSe_4$
$Li_2AuAlSe_4$	$K_2AlSbSe_4$	Co_2FeNiO_4	$Ag_2NiCrSe_4$
$Li_2CoTiSe_4$	$Li_2NaNbTe_4$	Pd_2FeZnS_4	Co_2NaGaO_4
$Li_2FeTiSe_4$	K_2AlSbS_4	Fe_2KInS_4	Ag_2ZnHfO_4
$Na_2MgTiSe_4$	$K_2InSbSe_4$	$Na_2ZnZrTe_4$	$Ag_2NaMoTe_4$
$Na_2FeCrSe_4$	$K_2MgTiTe_4$	$Na_2MgGeTe_4$	Li_2NiCTe_4
$Na_2FeGeSe_4$	Mg_2FeNiS_4	$Na_2AlGaTe_4$	Pt_2CoNiS_4
$Na_2CoHfTe_4$	Fe_2LiInO_4	K_2ZnCTe_4	Li_2FeCTe_4
$K_2PdTiSe_4$	Ag_2CoCS_4	Fe_2KGaO_4	$Fe_2MgNiTe_4$
K_2AlSbO_4	Mg_2FeCoS_4	Pd_2CoZnS_4	Li_2CoCTe_4
$Li_2PtSiSe_4$	Ag_2NiCS_4	$Ag_2FeHfSe_4$	Zn_2NaInS_4
$K_2CoSnSe_4$	Co_2KAuO_4	Pd_2LiAuO_4	$Li_2CoSiTe_4$
$Li_2MgSnSe_4$	Li_2KCrTe_4	$Pd_2MgZnSe_4$	$Co_2MgFeTe_4$
$K_2AgCrSe_4$	$Na_2LiCrTe_4$	Ag_2ZnZrO_4	$Ag_2LiNbTe_4$
$Na_2NiCrSe_4$	$Ag_2MgSiSe_4$	Pd_2NiZnS_4	$Fe_2NaAlSe_4$
$Na_2CoTiSe_4$	Ag_2CoCO_4	$Ag_2CoHfSe_4$	Mg_2NaGaO_4
$Na_2ZnCrSe_4$	Ag_2FeCO_4	$Li_2AgNbTe_4$	Ni_2KAuSe_4
K_2FeCSe_4	Pd_2NaAlS_4	$K_2ZnTiTe_4$	Zn_2KAlSe_4
$Na_2FeTiSe_4$	$Na_2AuSbSe_4$	Pd_2KGaO_4	Fe_2KAlSe_4
$Li_2NiTiSe_4$	Ag_2PdZrO_4	Ag_2MgCSe_4	Mg_2KGaO_4
K_2PtZrS_4	$Na_2PdSiTe_4$	Fe_2NaGaO_4	Pt_2FeNiS_4
$Na_2MgSnSe_4$	Ag_2NiCO_4	Fe_2LiGaO_4	$Ag_2NaNbTe_4$
Li_2MgCSe_4	$Li_2MgZrTe_4$	Zn_2CoNiS_4	$Na_2ZnSnTe_4$
$K_2FeSnSe_4$	Pd_2MgNiO_4	Ag_2KNbTe_4	$Mg_2FeCoTe_4$
$Na_2NiTiSe_4$	Ag_2CoHfS_4	Zn_2NaAlS_4	$Ni_2MgFeSe_4$
Na_2PtTiS_4	K_2GaSbS_4	$Na_2PtHfTe_4$	$Co_2MgNiSe_4$
$Li_2MgTiSe_4$	Ag_2FeHfS_4	Fe_2LiGaS_4	Co_2KGaO_4

Ag_2KMoS_4	Pd_2AgGaO_4	Fe_2MgZnO_4	$Na_2ZnTiTe_4$
$K_2ZnTiSe_4$	Ag_2PdGeO_4	$Ag_2PdHfSe_4$	$Mg_2FeNiTe_4$
$K_2ZnSnSe_4$	Fe_2KInO_4	Ag_2FeGeS_4	$Pd_2FeZnSe_4$
$Li_2GaInSe_4$	Fe_2NaAuS_4	$Ag_2NiHfSe_4$	Zn_2NaAlO_4
$Na_2PdSnSe_4$	Pd_2MgCoO_4	Fe_2KAlO_4	$Pd_2CoNiSe_4$
Na_2MgCSe_4	Mg_2CoNiO_4	$Ag_2ZnHfSe_4$	Co_2NaInO_4
$Na_2AuAlSe_4$	Ag_2PdCrS_4	Zn_2FeNiS_4	Fe_2NaSbS_4
K_2GaSbO_4	Mg_2FeNiO_4	Mg_2KAlS_4	Na_2ZnCTe_4
Na_2PtCSe_4	Ag_2NiSiO_4	Ni_2CoZnS_4	Fe_2KAlTe_4
$Na_2PtSiSe_4$	Mg_2FeCoO_4	$Pd_2NaGaSe_4$	$Ni_2MgCoSe_4$
$Na_2GaInSe_4$	Pd_2MgFeO_4	Zn_2FeCoS_4	$Ni_2LiAuSe_4$
$Li_2AuGaSe_4$	Ag_2CoSiO_4	$Zn_2MgPdSe_4$	Co_2PdPtS_4
Na_2InSbO_4	$K_2GaSbSe_4$	Co_2NiZnS_4	Zn_2LiGaO_4
$Li_2MgHfTe_4$	$Li_2GaSbSe_4$	Ni_2FeZnS_4	Fe_2PtZnS_4
K_2PtTiS_4	Ag_2FeSiO_4	$K_2AuInTe_4$	Ni_2CoPtS_4
$Na_2NiSnSe_4$	Ag_2MgCrO_4	Co_2NaAlO_4	$Ni_2NaAuSe_4$
$Li_2PtHfSe_4$	Ag_2PdTiS_4	Ag_2PdCSe_4	$Li_2NiSiTe_4$
Ag_2MgSiS_4	Ag_2PdTiO_4	$Li_2PdZrTe_4$	Pt_2KAuS_4
$Li_2PtGeSe_4$	$Pd_2AgAlSe_4$	Mg_2KGaS_4	Pd_2KAuS_4
$Na_2PdHfTe_4$	$K_2ZnGeTe_4$	Fe_2NiZnS_4	Co_2KInO_4
$Li_2NiSnSe_4$	Pd_2NaGaS_4	Co_2FeZnS_4	Pd_2FePtS_4
Ag_2NaMoS_4	$K_2MgSnTe_4$	Pd_2NaGaO_4	$Fe_2CoPdSe_4$
$Li_2FeSnSe_4$	Fe_2MgCoS_4	$Li_2ZnZrTe_4$	Fe_2AgAuS_4
Li_2AlSbS_4	Co_2MgFeO_4	Ag_2NiGeS_4	Pd_2CoPtS_4
$K_2NaCrTe_4$	$Mg_2FePdSe_4$	$Pd_2LiAlSe_4$	$Ag_2MgZrTe_4$
Na_2KNbTe_4	$Co_2LiAuSe_4$	Ag_2CoGeS_4	$Pd_2AgGaSe_4$
Ag_2KNbS_4	$Mg_2AgGaSe_4$	Fe_2LiAlO_4	$Ag_2PdGeSe_4$
$Na_2FeSnSe_4$	Pd_2FeNiO_4	Mg_2AgInS_4	$Fe_2NiPdSe_4$
$K_2LiNbTe_4$	Pd_2FeZnO_4	Fe_2CoZnS_4	$Co_2NaGaSe_4$

$Li_2CoSnSe_4$	$Mg_2CoPdSe_4$	Co_2KInSe_4	Ni_2FePtS_4
$Li_2PtSnSe_4$	Ag_2NiCrO_4	$Li_2AgMoTe_4$	Pd_2NaAuS_4
$Li_2AuInSe_4$	Fe_2LiInS_4	$Na_2AlInTe_4$	$Co_2FePdSe_4$
$Na_2PtHfSe_4$	$Mg_2PdZnSe_4$	$Co_2NaInSe_4$	$Ag_2FeGeSe_4$
Ag_2MgHfS_4	$Mg_2NiPdSe_4$	Co_2MgZnO_4	$Ag_2CoGeSe_4$
$Na_2CoSnSe_4$	Pd_2CoZnO_4	$Na_2MgTiTe_4$	$Mg_2NaInSe_4$
$Li_2PdSnSe_4$	$Mg_2AgAlSe_4$	$Li_2FeSnTe_4$	$Mg_2AgInSe_4$
Na_2AlSbS_4	Fe_2MgNiO_4	Fe_2NaAlO_4	$Pd_2CoZnSe_4$
$K_2AuAlSe_4$	$K_2PtZrSe_4$	$Li_2NiZrTe_4$	$Co_2MgZnSe_4$
Ag_2KCrS_4	Ni_2MgFeS_4	Co_2NaInS_4	Co_2NiPtS_4
$K_2PtSiSe_4$	Pd_2MgZnO_4	Zn_2AgGaS_4	Pt_2FePdS_4
$K_2NiHfTe_4$	Pd_2NiZnO_4	$Li_2PdTiTe_4$	$Pd_2NiZnSe_4$
Li_2GaSbS_4	Co_2NaAuO_4	Zn_2KGaS_4	$Fe_2MgPdTe_4$
$K_2LiMoTe_4$	Ag_2ZnCrO_4	$Li_2AlInTe_4$	Pt_2FeCoS_4
$K_2ZnHfTe_4$	Pd_2LiGaS_4	Ag_2FeCSe_4	$Fe_2LiGaSe_4$
Ag_2MgZrS_4	Fe_2MgNiS_4	$Li_2PdCrTe_4$	$Ni_2FePdSe_4$
K_2PtCSe_4	$Ag_2PdSiSe_4$	Zn_2NaGaS_4	Mg_2KInS_4
$K_2CoHfTe_4$	Co_2MgNiS_4	Co_2LiAlS_4	$Co_2LiGaSe_4$
$K_2PdHfTe_4$	Ni_2MgCoS_4	Ni_2KInS_4	Zn_2KAlO_4
K_2InSbO_4	Pd_2LiAlO_4	$Mg_2FeZnSe_4$	$Mg_2FePdTe_4$
$K_2FeHfTe_4$	$Na_2FeZrTe_4$	$Li_2AgCrTe_4$	$Mg_2NaAlSe_4$
$Na_2PtSnSe_4$	$Na_2NiZrTe_4$	$Mg_2CoNiSe_4$	$Fe_2NaGaSe_4$
$Na_2ZnHfTe_4$	$Na_2CoSiTe_4$	Zn_2LiGaS_4	Zn_2LiInS_4
$Li_2ZnTiSe_4$	$Na_2NiSiTe_4$	$Li_2FeZrTe_4$	$Co_2NiPdSe_4$
$Na_2AuInSe_4$	Pd_2KAlS_4	Fe_2KSbS_4	$Li_2ZnTiTe_4$
$Na_2ZnTiSe_4$	Pd_2CoNiO_4	$Li_2PdSiTe_4$	Pd_2KSbS_4
Na_2KMoTe_4	$K_2ZnZrTe_4$	Ni_2LiAlS_4	$Ag_2NiTiSe_4$
$Na_2PtGeSe_4$	$Na_2CoZrTe_4$	$Li_2CoSnTe_4$	$Ni_2NaAlSe_4$
$Na_2AuGaSe_4$	Ag_2MgHfO_4	$Mg_2FeNiSe_4$	$Ag_2FeTiSe_4$

$Ag_2NaMoSe_4$	Fe_2MgCoO_4	$Mg_2FeCoSe_4$	$Zn_2MgFeSe_4$
$Li_2ZnSnSe_4$	Co_2MgFeS_4	$Na_2AuInTe_4$	Ag_2PtHfS_4
Ag_2NaNbS_4	Co_2LiAuO_4	$Na_2PtSnTe_4$	$Ag_2CoTiSe_4$
$K_2PtHfSe_4$	$Na_2FeSiTe_4$	Ni_2NaInS_4	Pd_2KInO_4
Ag_2KMoO_4	Co_2FePdS_4	Ag_2CoCSe_4	$Ag_2NiGeSe_4$
Ag_2NaCrS_4	Fe_2NiPdS_4	$Li_2MgSnTe_4$	$Ni_2LiInSe_4$
$K_2MgZrTe_4$	$K_2AgNbTe_4$	$Li_2ZnSiTe_4$	Fe_2KAuTe_4
$K_2ZnSiTe_4$	Ni_2FePdS_4	$Mg_2CoZnSe_4$	$Ni_2NaInSe_4$
Li_2InSbS_4	Pd_2NaAlO_4	$Mg_2NiZnSe_4$	$Pt_2NaAuSe_4$
$Li_2NiHfTe_4$	Co_2NiPdS_4	Mg_2LiAlS_4	Ni_2KAlSe_4
$K_2AuInSe_4$	Ag_2PdZrS_4	Ni_2MgZnO_4	$Pd_2NaAuSe_4$
Ag_2KCrSe_4	$K_2CoZrTe_4$	Pd_2LiInS_4	Pd_2NaInO_4
Ag_2LiMoS_4	$K_2NiZrTe_4$	Ag_2NiCSe_4	Pt_2KAuSe_4
Ag_2KNbO_4	$Na_2AgNbTe_4$	Ni_2LiAlO_4	$Ni_2MgZnSe_4$
$Li_2FeHfTe_4$	$K_2PdZrTe_4$	Zn_2MgFeO_4	Fe_2LiSbS_4
$K_2PtSnSe_4$	$K_2AgMoTe_4$	$Li_2NiSnTe_4$	$Fe_2PdZnSe_4$
$Li_2CoHfTe_4$	Ag_2NiZrS_4	$Li_2CoZrTe_4$	Pt_2NaAuS_4
Zn_2MgPdO_4	Ag_2CoZrS_4	$Fe_2NaInSe_4$	$Fe_2AgAlTe_4$
Li_2KNbTe_4	$Fe_2AgAlSe_4$	$Pd_2LiGaSe_4$	$Pd_2LiAuSe_4$
$Na_2LiNbTe_4$	Ag_2ZnCS_4	$Li_2MgGeTe_4$	Ag_2GaInS_4

Supplementary Figures

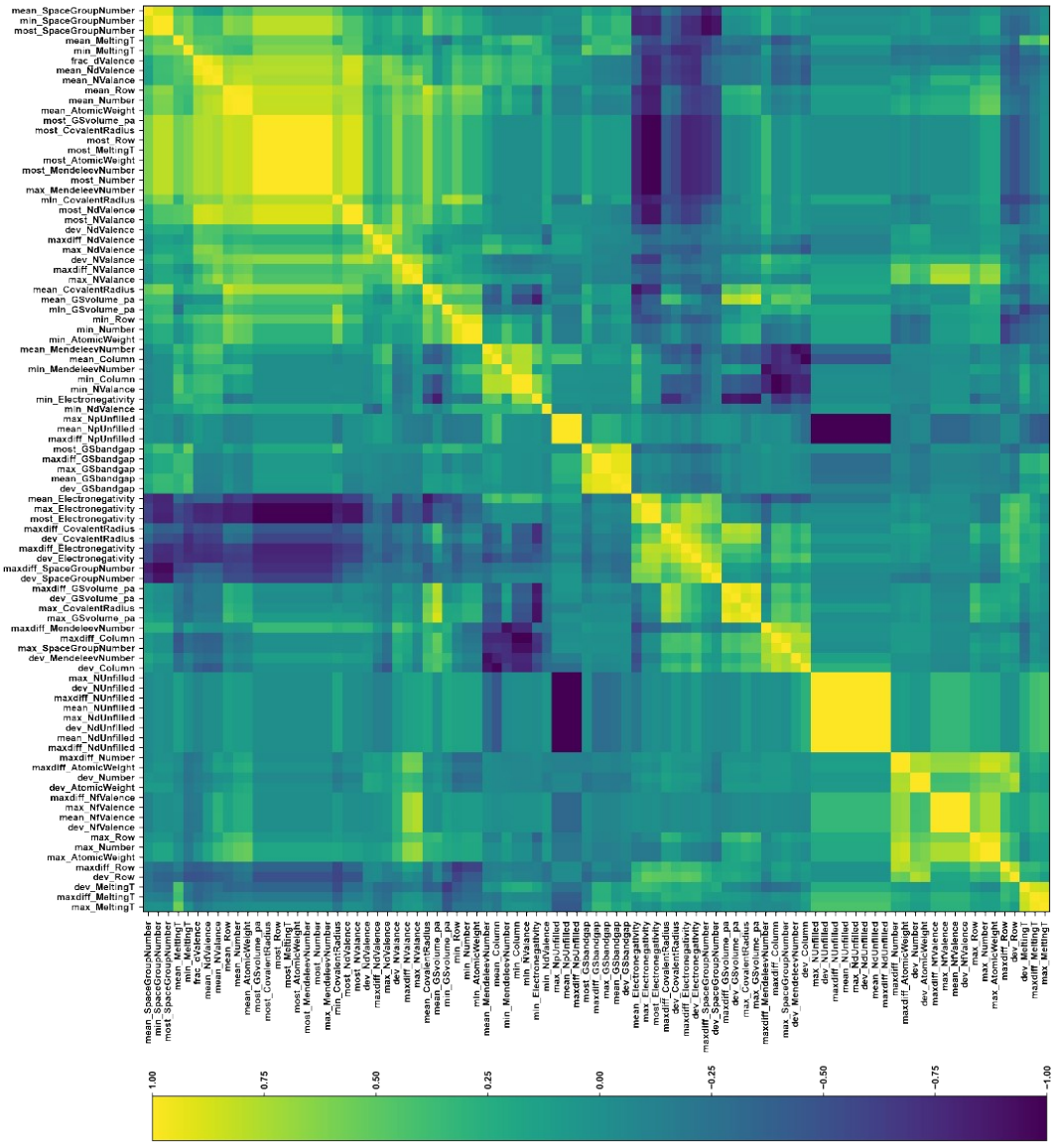

Fig. S1. The Person correlation heat map of the initial 145 feature descriptors. The numbers in the heat map represent the correlations among these features. Yellow represents positive correlations, and purple represents negative correlations. The features with an absolute correlation value greater than 0.8 and low rank of importance were deleted.

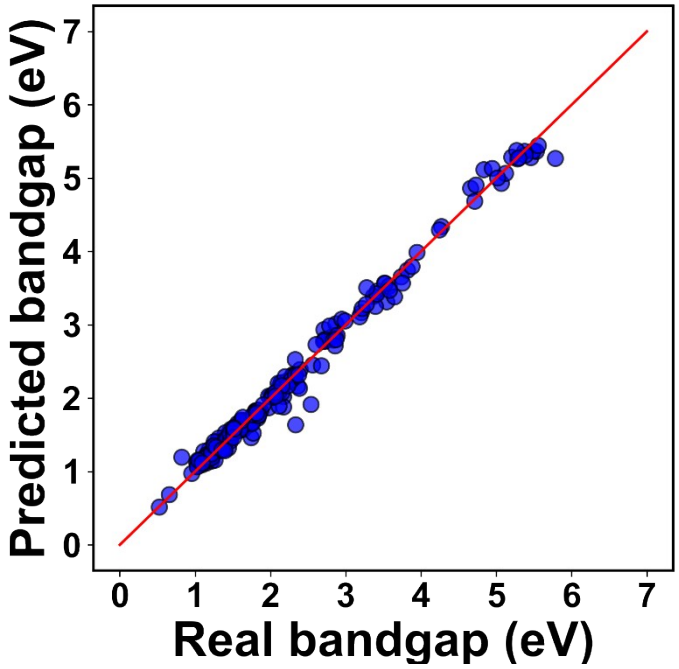

Fig. S2. Validation set fitting results of the bandgaps predicted by ML and real DFT calculations searched by literatures.

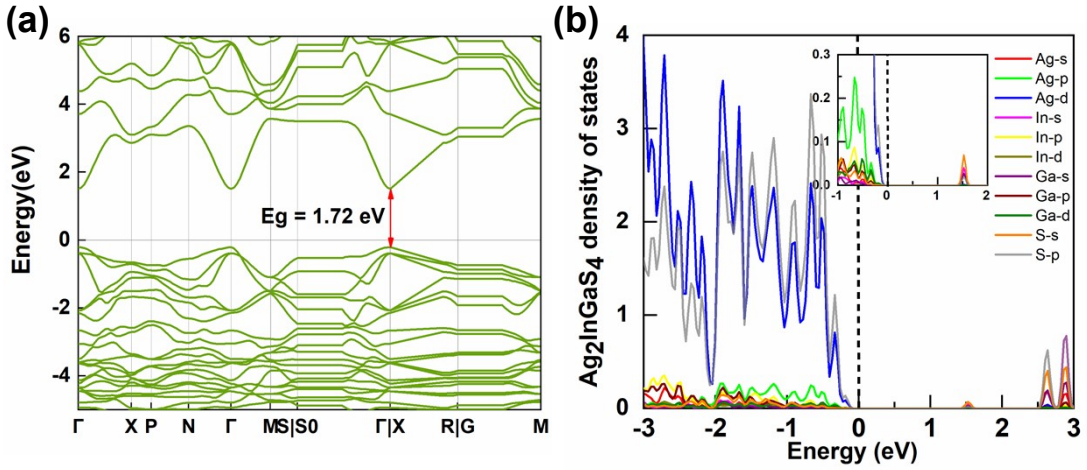

Fig. S3. DFT calculation results for Ag_2InGaS_4. (a) The electronic band structure calculated with HSE and (b) the Projected density of states for Ag_2InGaS_4.

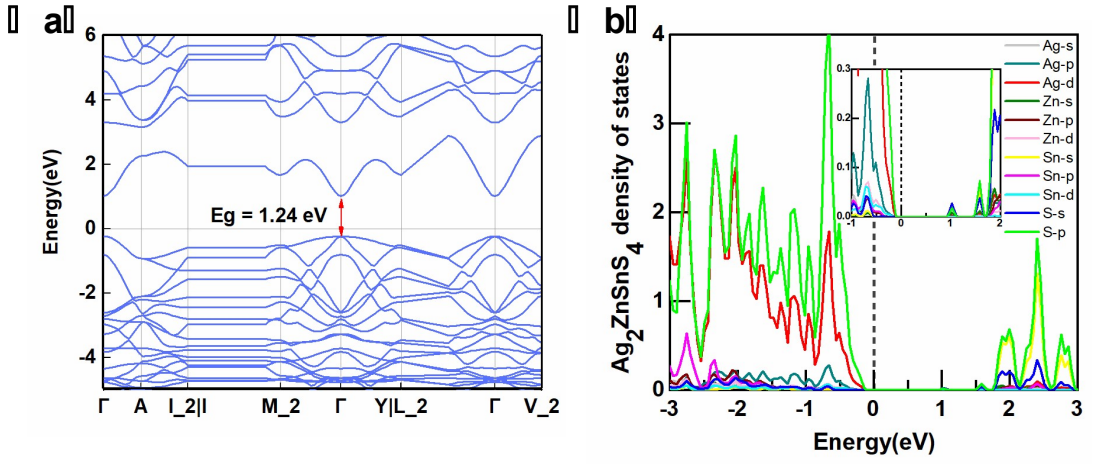

Fig. S4. DFT calculation results for Ag_2ZnSnS_4. (a) The electronic band structure calculated with HSE and (b) the Projected density of states for Ag_2ZnSnS_4.

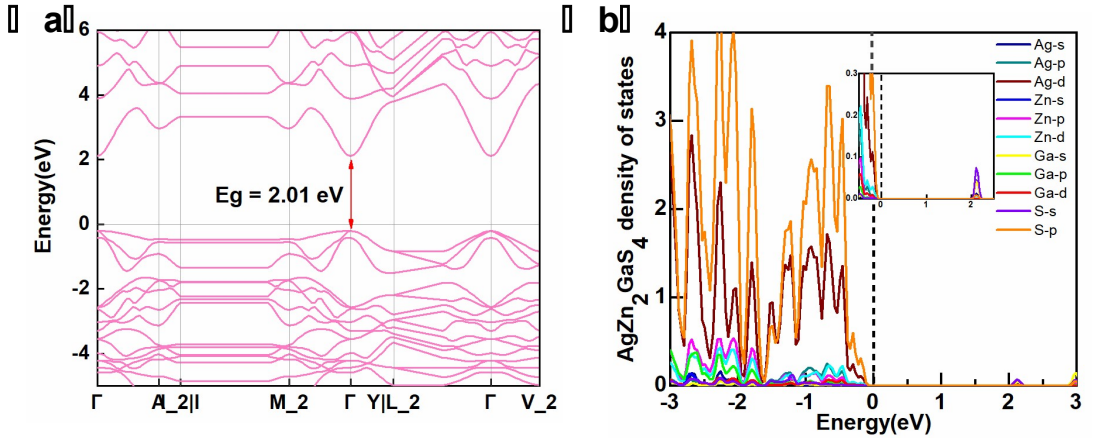

Fig. S5. DFT calculation results for $AgZn_2GaS_4$. (a) The electronic band structure calculated with HSE and (b) the Projected density of states for $AgZn_2GaS_4$.

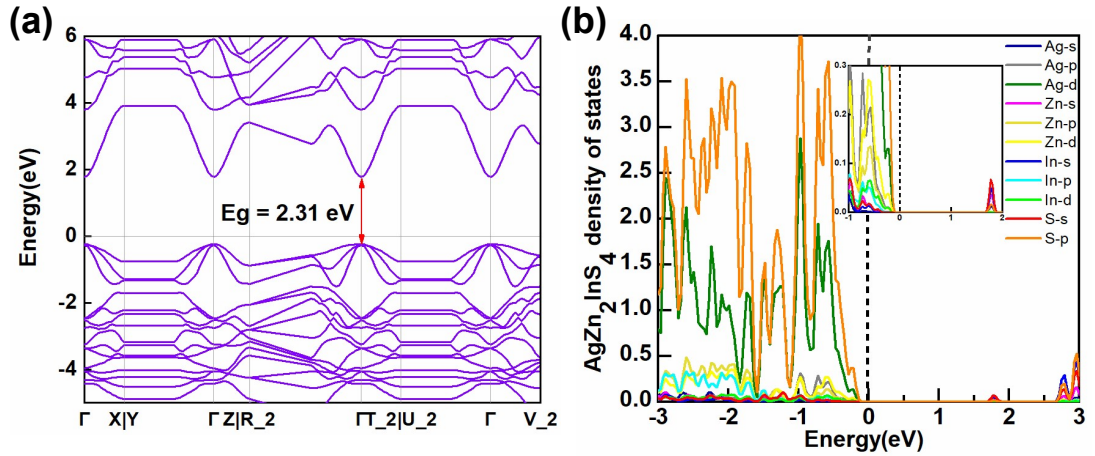

Fig. S6. DFT calculation results for $AgZn_2InS_4$. (a) The electronic band structure calculated with HSE and (b) the Projected density of states for $AgZn_2InS_4$.

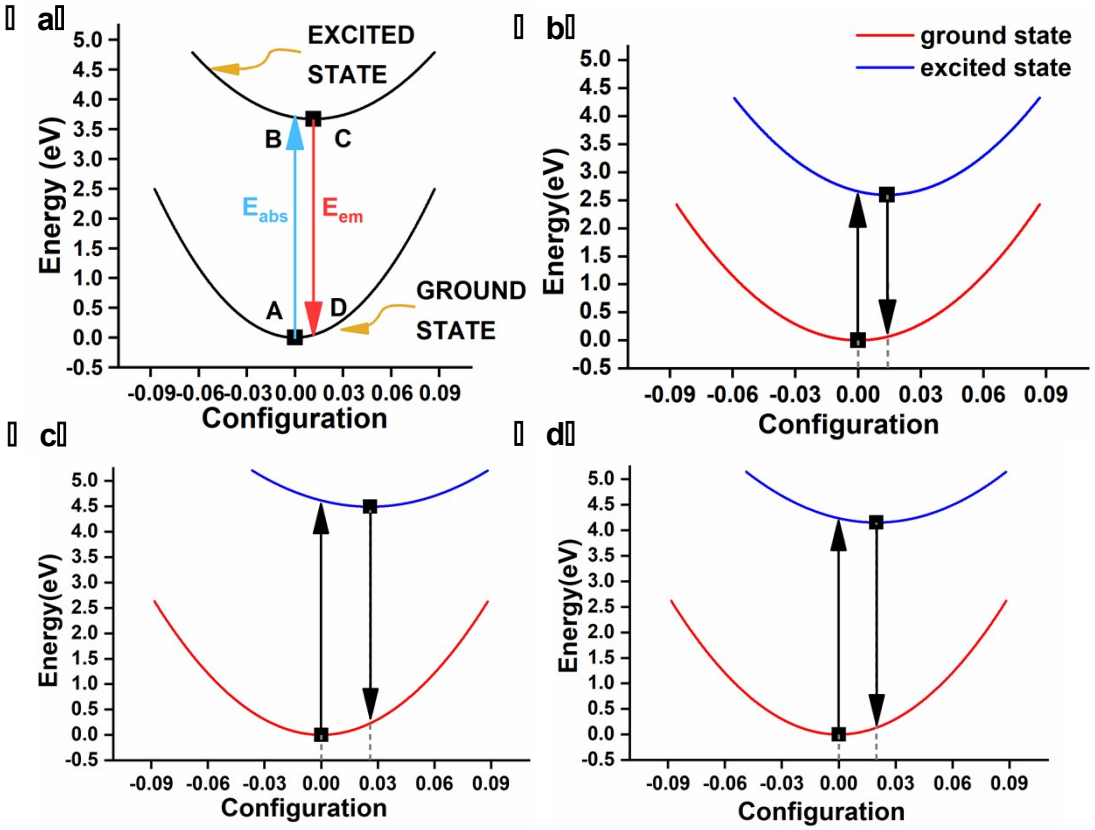

Fig. S7. The configuration coordinate diagram describing the luminescence center of (a) Ag2InGaS4, (b) Ag_2ZnSnS_4, (c) $AgZn_2GaS_4$, (d) $AgZn_2InS_4$.