SUPPLEMENTARY INFORMATION

Investigation of thermal control in phase-changing ABO_3 perovskites via first-principles predictions: General mechanism of emittance

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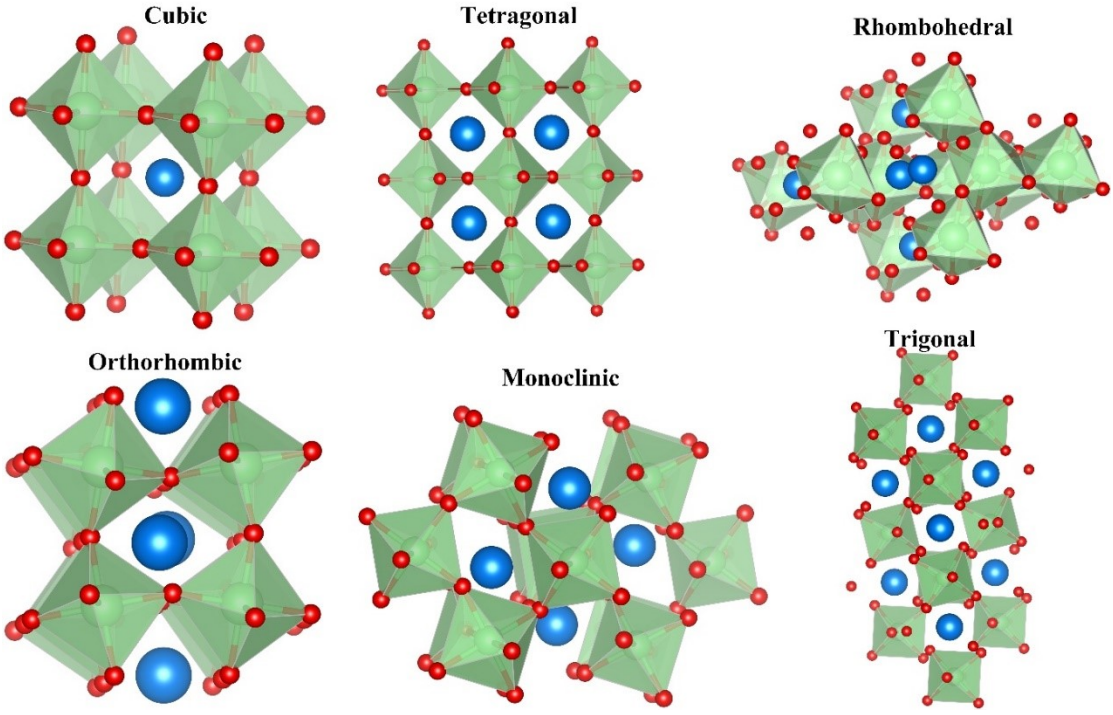

Fig. S1. Fragment of the crystal structures of the ideal orthorhombic, cubic, monoclinic, tetragonal, trigonal and rhombohedral perovskites. A cation is blue ball, B cation is green ball and the cornersharing BO_6 octahedra is reseda network.

Compounds		Crystal											
		Cubic, Pm3m	Orthorhombic, Pnma	Orthorhombic, IMMA	Orthorhombic, Pbnm	Orthorhombic, Cmcm	Orthorhombic, Pba2	Tetragonal, I4/mcm	Monoclini, Pn/21	Rhombohedral, R3c	Triclinic, P1	Trigonal, R3c	Hexhagonal, P63cm
$ANiO_3$	A=La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Y		√						√				
$DNbO_3$	D=Ag, Ba, Ca, Eu, Pr,Sr	√	√					√					
	D=K, Na	√	√						√				
	D=Li	√	√										
$MSnO_3$	M=Hg, Mg, Ni, Sr, Zn, Ba	√	√					√					
	M=Ca, Cd, Co, Fe, Mn, Ti, V	√	√					√		√			
$EuBO_3$	B=Hf, Ti, Zr	√	√					√					
$XTaO_3$	X=Li, Na, K, Ag	√	√					√					
$ETiO_3$	E=Ti	√	√					√					
	E=Mn	√	√							√			
	E=Mg	√	√										
	E=Sr	√	√					√		√			
	E=Pb	√						√					
$GZrO_3$	G=Ba	√						√					
	G=Ca	√	√				√						
$LaTM^2O_3$	TM^2=Cr, Ga	√	√									√	
	TM^2=Ti, Sc	√	√		√								
	TM^2=Fe	√	√				√					√	
	TM^2=Co	√	√					√	√		√	√	
	TM^2=Al	√		√		√		√	√		√	√	√
	TM^2=V	√	√										
$ZFeO_3$	Z=Ba, Lu	√	√					√		√			
$SrTM^1O_3$	TM^1=Mo	√	√					√	√				
	TM^1=Zr	√		√		√		√					
	TM^1=Hf	√	√	√				√					
	TM^1=Ru	√	√					√					
	TM^1=Cr	√	√										√
	TM^1=Tc	√		√									
YTM^3O_3	TM^3=Co	√	√									√	√
	TM^3=Cr, Fe, Ti	√	√										√
	TM^3=V		√					√					√
$NaOsO_3$		√		√								√	
$BaPbO_3$			√							√			

Fig. S2 The calculated crystal structure of 76 kinds of ABO_3 perovskites in this work.

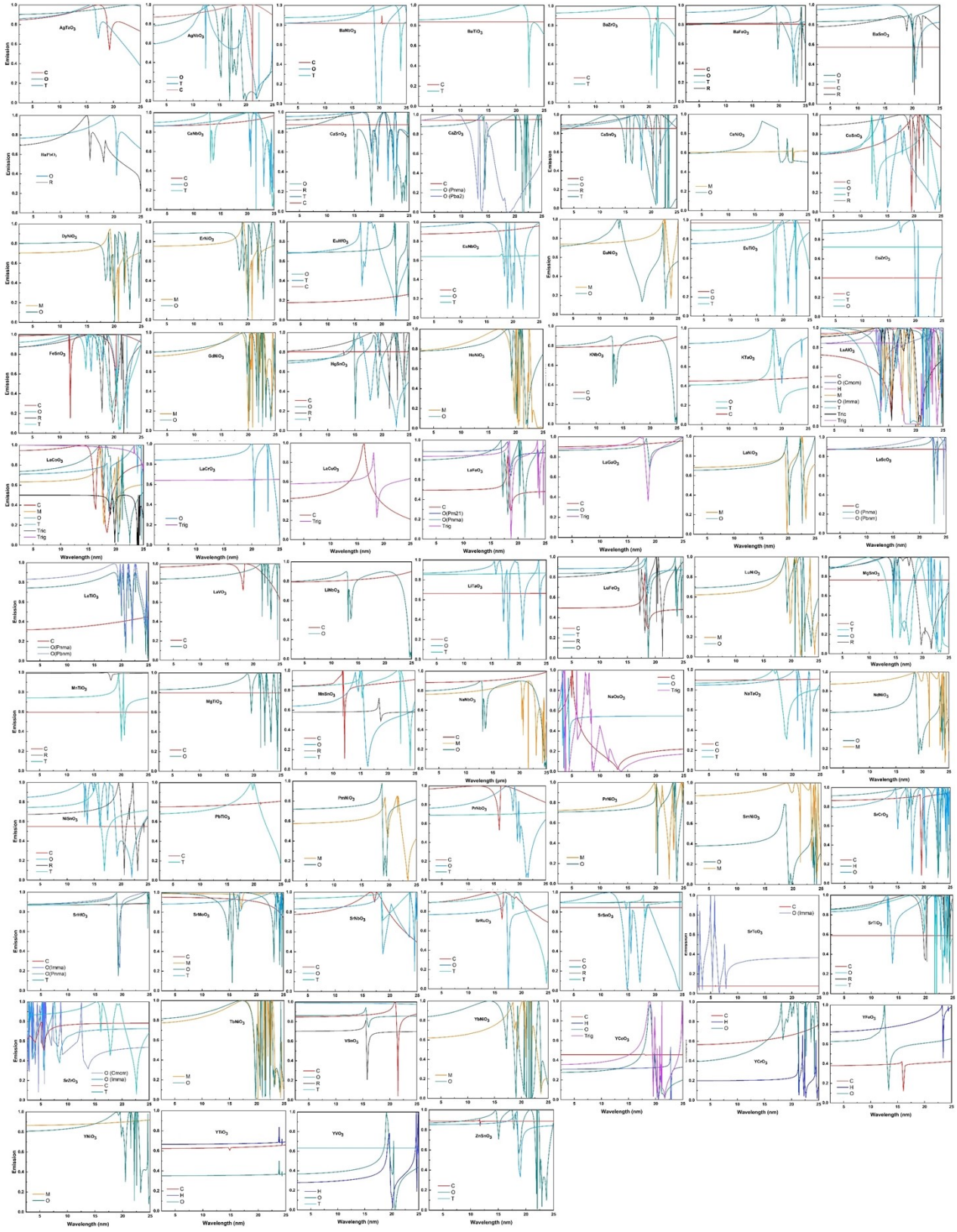

Fig. S3 MIR emission spectrum (2-25μm) of 76 kinds of ABO_3.

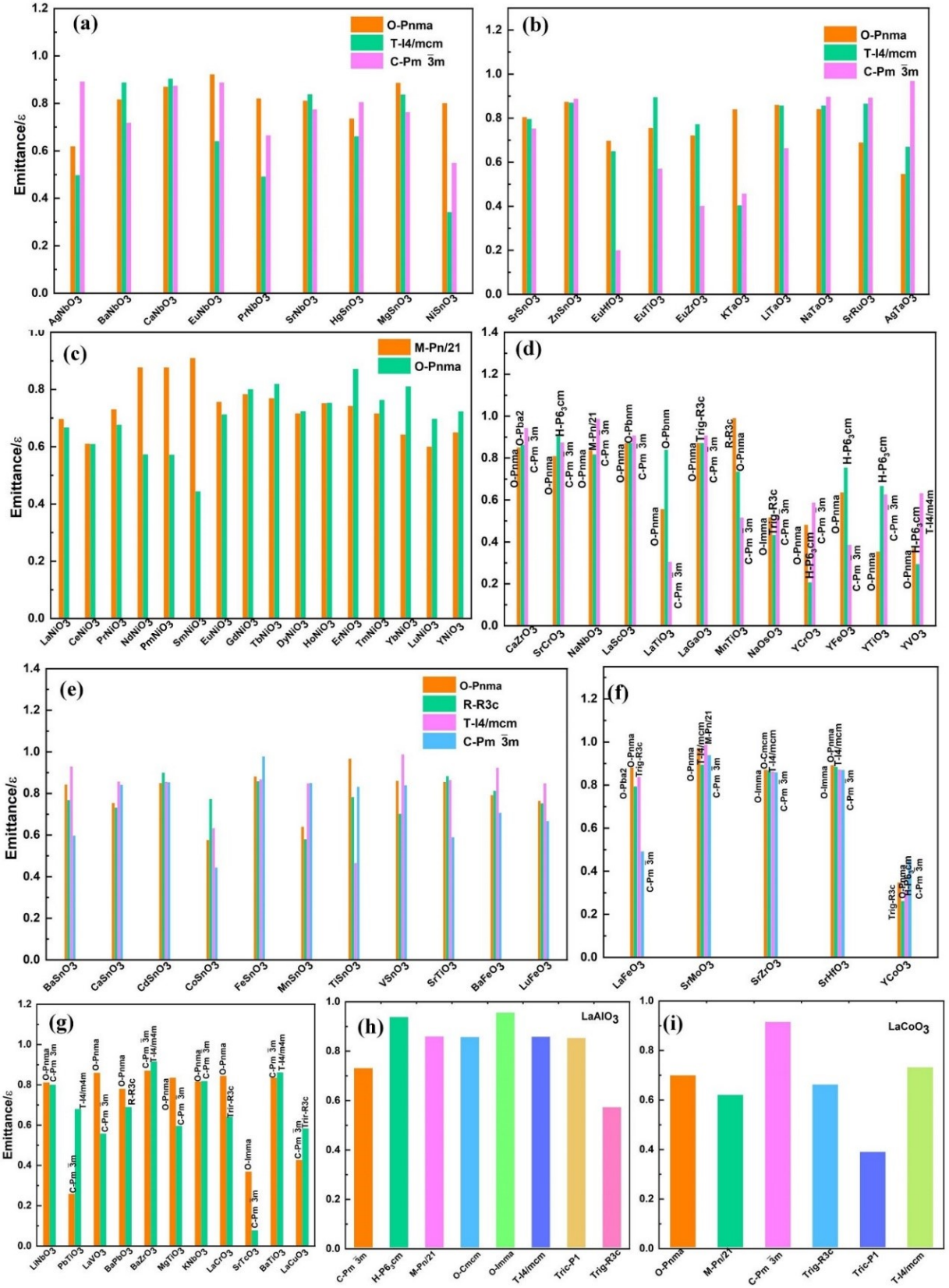

Fig. S4 Average MIR emissivity (2-25μm) of 76 kinds of ABO_3.

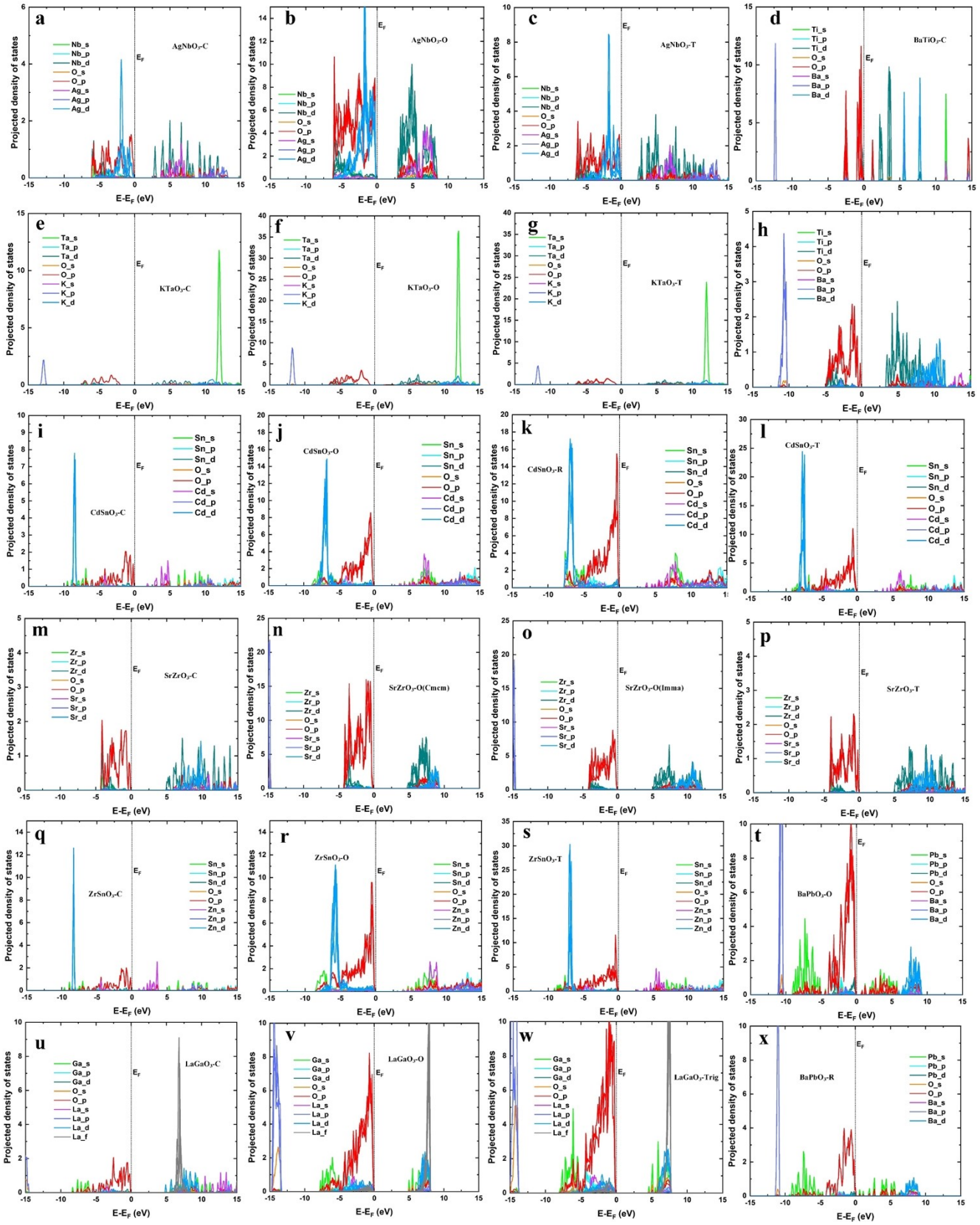

Fig. S5 Projected density of states of band insulators $AgNbO_3$, $BaTiO_3$, $KTaO_3$, $CdSnO_3$, $ZnSNO_3$, $SrZrO_3$, $LaGaO_3$, $BaPbO_3$.

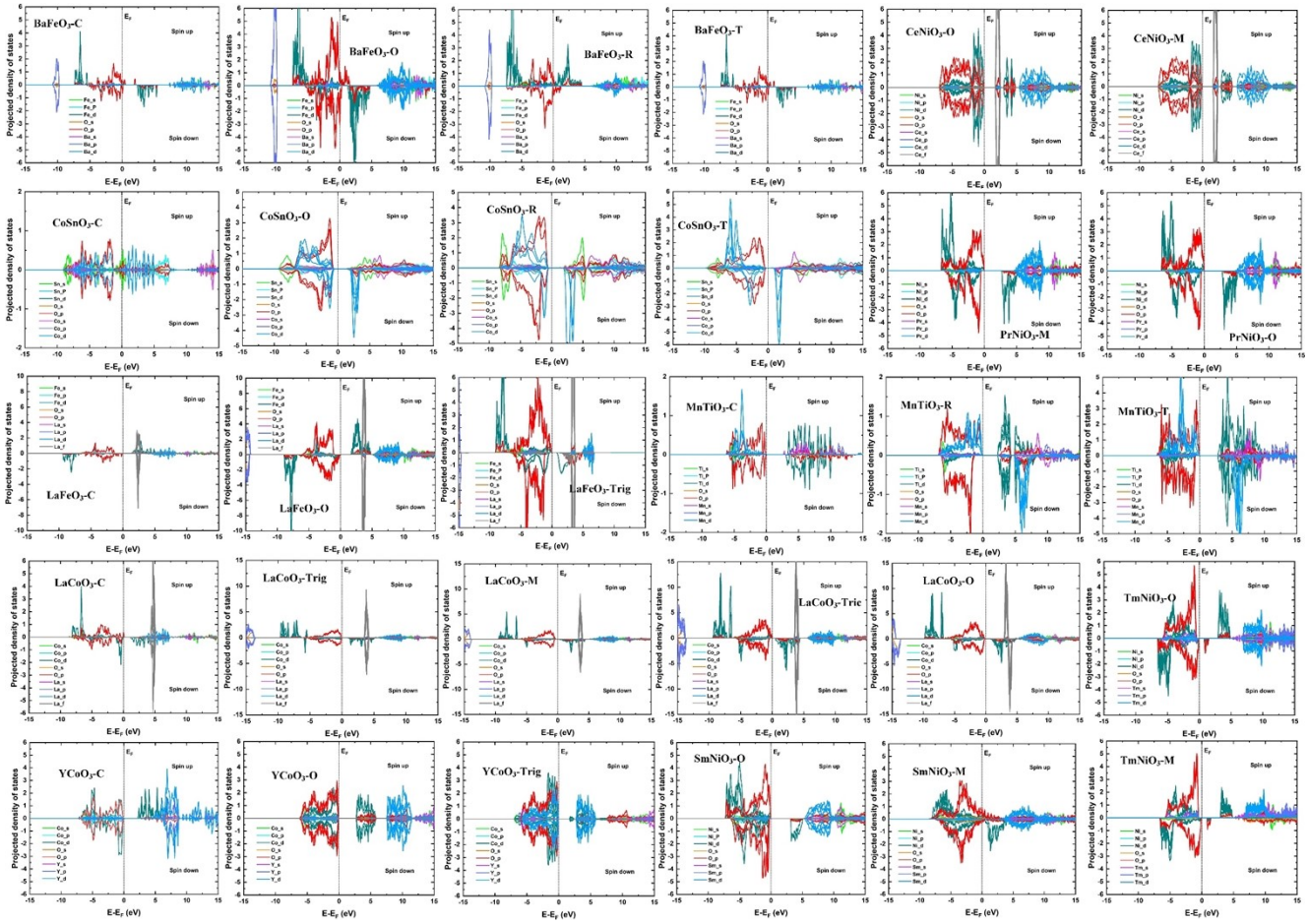

Fig. S6 Projected density of states of $CeNiO_3$, $TmNiO_3$, $PrNiO_3$, $SmNiO_3$, $BaFeO_3$, $LaFeO_3$, $LaCoO_3$, $CoSnO_3$, $MnTiO_3$, and $YCoO_3$.

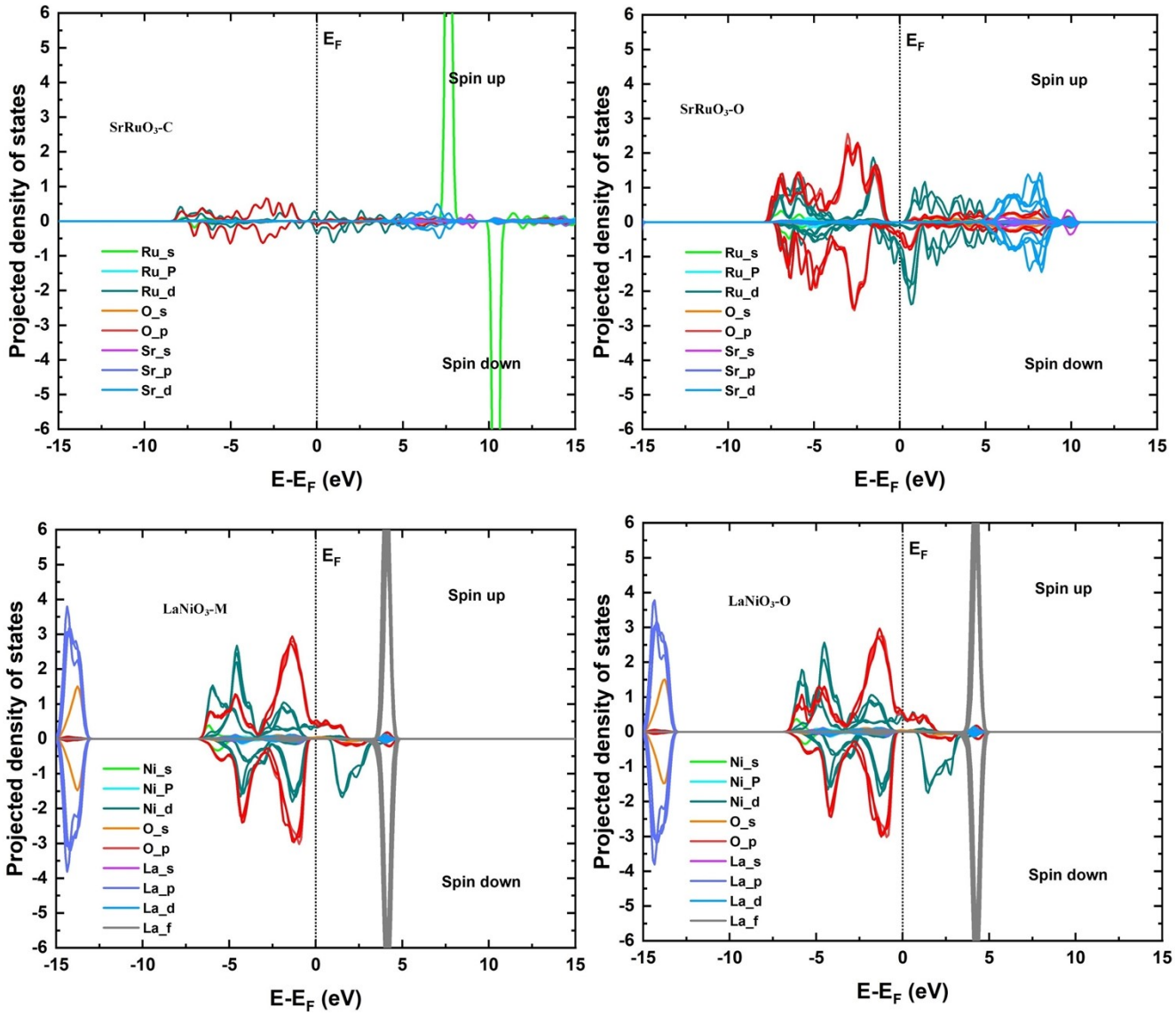

Fig. S7 Projected density of states of metals $SrRuO_3$ and $LaNiO_3$.