Supporting Information

‘Synthesis, Crystal structure, and Optical properties of Layered Perovskite Scandium Oxychlorides: Sr_2ScO_3Cl, $Sr_3Sc_2O_5Cl_2$, and $Ba_3Sc_2O_5Cl_2$’

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Table S1. Anisotropic displacement parameters for Sr_2ScO_3Cl.

Atom	U_{11}/Å^2	U_{22}/Å^2	U_{33}/Å^2
Sr1	0.0100(2)	0.0100(2)	0.0077(2)
Sr2	0.00314(14)	0.00314(14)	0.0121(2)
Sc	0.00590(8)	0.00590(8)	0.0099(2)
O_{eq}	0.0068(2)	0.0021(2)	0.00138(2)
O_{ap}	0.0219(2)	0.0219(2)	0.055(3)
Cl	0.01078(11)	0.01078(11)	0.0129(2)

Table S2. Anisotropic displacement parameters for $Sr_3Sc_2O_5Cl_2$.

Atom	U_{11}/Å^2	U_{22}/Å^2	U_{33}/Å^2
Sr1	0.0137(3)	0.0137(3)	0.0219(5)
Sr2	0.0051(2)	0.0051(2)	0.0084(3)
Sc	0.00622(9)	0.00622(9)	0.0098(2)
O_{eq}	0.0064(2)	0.0020(2)	0.0241(3)
O_{ap}	0.0336(4)	0.0336(4)	0.0056(6)
Cl	0.01185(13)	0.01185(13)	0.0140(2)

Table S3. Anisotropic displacement parameters for $Ba_3Sc_2O_5Cl_2$.

Atom	U_{11}/Å ^{2}	U_{22}/Å ^{2}	U_{33}/Å ^{2}
Ba1	0.0060(3)	0.0060(3)	0.0072(6)
Ba2	0.0030(2)	0.0030(2)	0.0074(3)
Sc	0.00663(7)	0.00663(7)	0.0094(2)
O_{eq}	0.0062(2)	0.0036(2)	0.0108(2)
O_{ap}	0.0127(2)	0.0127(2)	0.0017(4)
Cl	0.01054(14)	0.01054(14)	0.0152(2)

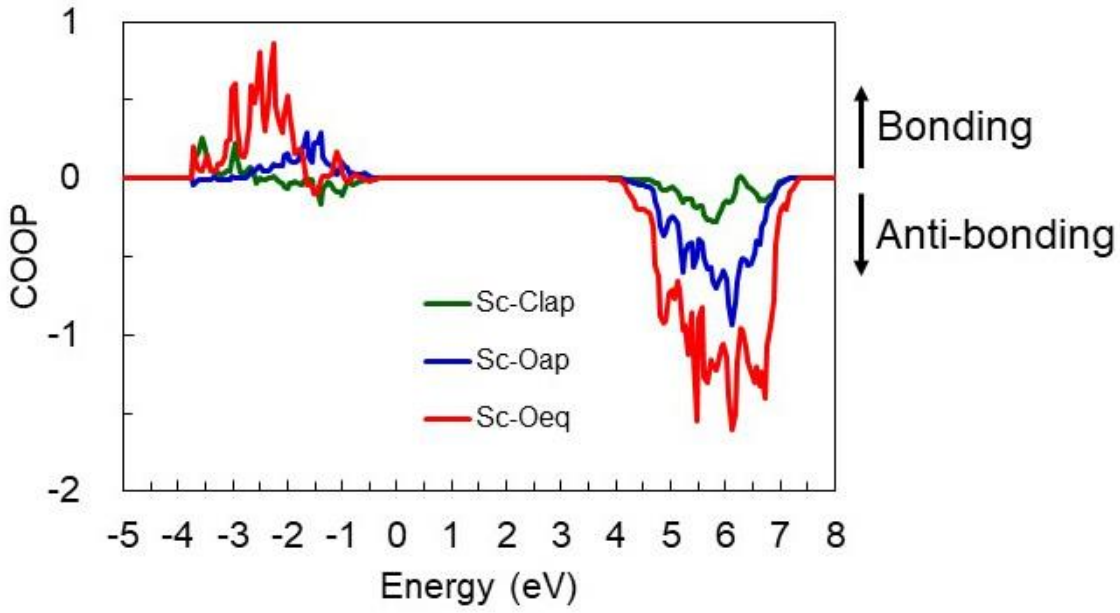

Figure S1. Crystal orbital overlap population (COOP) for Sc–O_{eq}, Sc–O_{ap}, and Sc–Cl_{ap} interactions in Sr_2ScO_3Cl. The COOP curves below the Fermi level show bonding states between Sc 3*d* and O2*p* orbitals but anti-bonding states between Sc 3*d* and Cl_{ap} 3*p* orbitals.

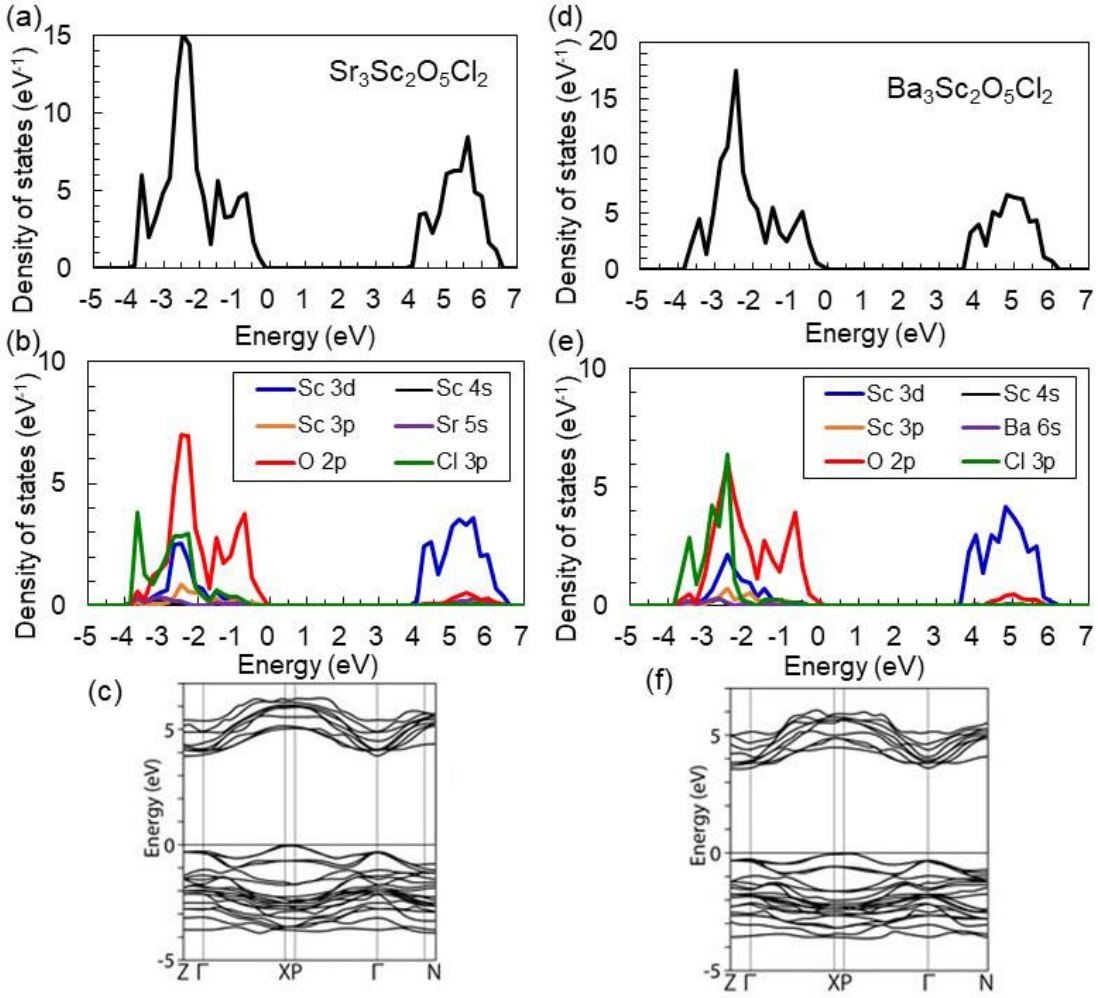

Figure S2. Total and partial density-of-states, and band dispersions of (a)-(c) $Sr_3Sc_2O_5Cl_2$ (d)-(f) $Ba_3Sc_2O_5Cl_2$.