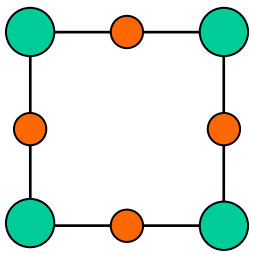
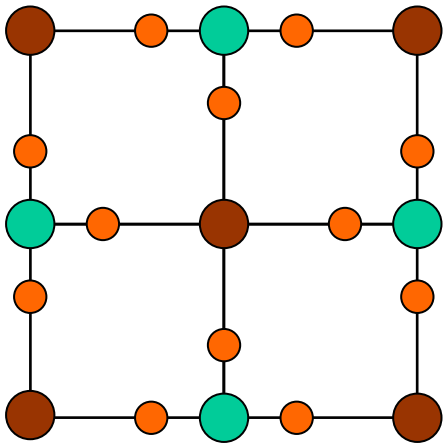
Class 5: Ordered double perovskites or elpasolites

Elpasolite and cryolite are the halide minerals with the ordered double perovskite structure. The formulae are K_2NaAlF_6 and $Na_2NaAlFe_6$ as well as variants thereof. Cryolite [Na_2NaAlF_6] is well known from its use as a solvent in the Hall-Héroult process of extracting Al from Al_2O_3 electrochemically.



perovskite



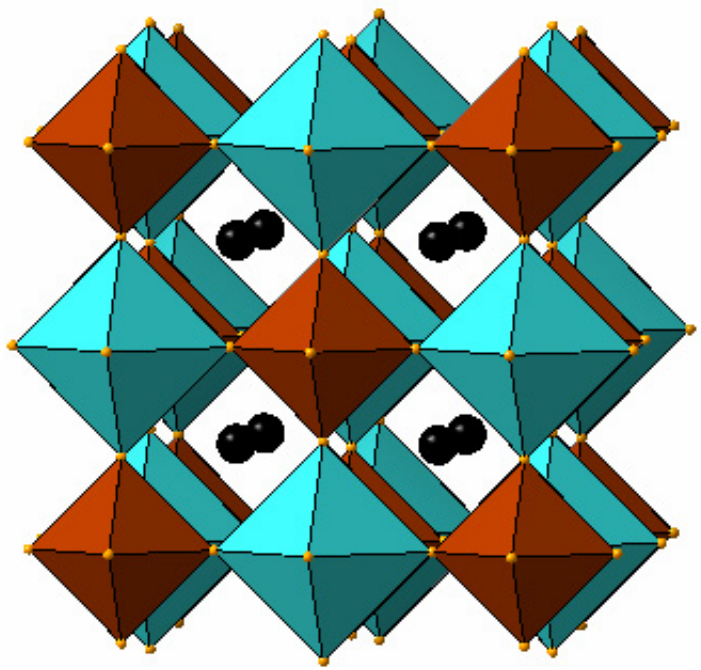
elpasolite

two different B cations:
$A_2BB'O_6$
$a = 2a_p = 8$ Å *Fm-3m*

A at (¼ ¼ ¼)
B at (0 0 0)
B′ at (½ ½ ½)
O at (x 0 0); x ~ ¼

Class 5: Ordered double perovskites or elpasolites

A typical oxide double perovskite Ba_2MgWO_6: The larger octahedra surround Mg^{2+}



Typically rather large differences in charge are required for the B and B′ to be fully ordered. Some ions tend to order easily (eg. Mn^{3+}, Cu^{2+}, while some others such as Cr^{3+} do not.

The standard reference is:
M. T. Anderson, K. B. Greenwood, G. A. Taylor, and K. R. Poeppelmeier, Prog. Solid State Chem. **22** (1993) 197. LINK

Class 5: Ordered double perovskites or elpasolites

Rock Salt

No.	compound	Δ IR
1.	Ba_2PrPtO_6	0.100

Rock Salt

No.	compound	Δ IR	comments
1.	A_2AlNbO_6	0.115	A = Ca, Sr
2.	A_2AlTaO_6	0.115	A = Ca, Sr
3.	A_2CrMoO_6	0.005	A = Ca, Sr
4.	A_2CrOsO_6	0.040	A = Ca, Sr
5.	A_2CrReO_6	0.035	A = Ca, Sr
6.	A_2CrWO_6	0.005	A = Ca, Sr
7.	A_2DyNbO_6	0.272	A = Ca, Sr, Ba
8.	A_2DyTaO_6	0.272	A = Ca, Sr, Ba
9.	A_2ErNbO_6	0.250	A = Ca, Sr, Ba
10.	A_2ErTaO_6	0.250	A = Ca, Sr, Ba
11.	A_2FeMoO_6	0.035	A = Ca, Sr, Ba
12.	A_2FeSbO_6	0.050	A = Ca, Sr
13.	A_2FeUO_6	0.205	A = Sr, Ba
14.	A_2GdNbO_6	0.298	A = Ca, Sr
15.	A_2GdTaO_6	0.298	A = Ca, Sr, Ba
16.	A_2HoNbO_6	0.261	A = Ca, Sr
17.	A_2HoTaO_6	0.261	A = Ca, Sr, Ba
18.	A_2InNbO_6	0.160	A = Ca, Sr, Ba
19.	A_2InOsO_6	0.225	A = Sr, Ba
20.	A_2InReO_6	0.220	A = Sr, Ba
21.	A_2InTaO_6	0.160	A = Ca, Sr, Ba
22.	A_2InUO_6	0.040	A = Sr, Ba
23.	A_2LaNbO_6	0.392	A = Ca, Ba
24.	A_2LaTaO_6	0.392	A = Ca, Ba
25.	A_2LuNbO_6	0.221	A = Sr, Ba
26.	A_2LuRuO_6	0.296	A = Sr, Ba
27.	A_2MnUO_6	0.205	A = Sr, Ba
28.	A_2NdNbO_6	0.343	A = Ca, Ba
29.	A_2NdTaO_6	0.343	A = Sr, Ba
30.	A_2PrNbO_6	0.350	A = Ca, Ba
31.	A_2PrTaO_6	0.350	A = Ca, Sr, Ba
32.	A_2ScOsO_6	0.170	A = Sr, Ba
33.	A_2ScReO_6	0.165	A = Ca, Sr, Ba
34.	A_2SmNbO_6	0.318	A = Ca, Sr, Ba
35.	A_2SmTaO_6	0.318	A = Ca, Sr, Ba
36.	A_2TbNbO_6	0.283	A = Ca, Sr
37.	A_2TbTaO_6	0.283	A = Ca, Sr, Ba
38.	A_2TmNbO_6	0.240	A = Sr, Ba
39.	A_2YNbO_6	0.260	A = Ca, Ba
40.	A_2YRuO_6	0.335	A = Ca, Sr, Ba
41.	A_2YTaO_6	0.260	A = Ca, Ba
42.	A_2YbNbO_6	0.228	A = Ca, Ba
43.	A_2YbTaO_6	0.228	A = Ca, Ba

Rock Salt

No.	compound	Δ IR	comments
44.	Ba_2BiBiO_6	0.270	
45.	Ba_2BiDyO_6	0.152	
46.	Ba_2BiSbO_6	0.160	
47.	Ba_2BiYO_6	0.140	
48.	Ba_2CrUO_6	0.225	
49.	Ba_2ErUO_6	0.050	
50.	Ba_2EuTaO_6	0.307	
51.	Ba_2GdSbO_6	0.338	
52.	Ba_2InSbO_6	0.200	tentative
53.	Ba_2LaRuO_6	0.467	
54.	Ba_2LuTaO_6	0.221	
55.	Ba_2RhNbO_6	0.040	
56.	Ba_2ScNbO_6	0.126	
57.	Ba_2ScSbO_6	0.145	
58.	Ba_2ScTaO_6	0.105	
59.	Ba_2ScUO_6	0.095	
60.	Ba_2YUO_6	0.080	
61.	Ca_2CrNbO_6	0.025	
62.	Ca_2CrTaO_6	0.025	
63.	Ca_2FeNbO_6	0.005	
64.	Ca_2FeTaO_6	0.005	
65.	$CaLaCaRuO_6$	0.435	
66.	La_2CoIrO_6	0.120	
67.	La_2CuMnO_6	0.070	
68.	La_2MgIrO_6	0.090	tentative
69.	Ln_2CuIrO_6	0.025	Ln = La, Nd
70.	Nd_2MgTiO_6	0.115	
71.	Pb_2InNbO_6	0.160	
72.	Pb_2ScTaO_6	0.105	
73.	Pb_2YbNbO_6	0.228	
74.	Sr_2CoSbO_6	0.010	
75.	Sr_2CrNbO_6	0.025	
76.	Sr_2CrSbO_6	0.015	
77.	Sr_2EuNbO_6	0.307	
78.	Sr_2GaReO_6	0.040	
79.	Sr_2GaSbO_6	0.020	
80.	Sr_2MnMoO_6	0.035	
81.	Sr_2RhSbO_6	0.080	

Charge diff. 1 and 2

Rock Salt

No.	compound	Δ IR	comments
1.	$ALaLiWO_6$	0.140	A = Sr, Ba
2.	$BaLaKWO_6$	0.840	
3.	$BaLaLiMoO_6$	0.170	
4.	$BaLaNaWO_6$	0.400	
5.	$SrLaNaUO_6$	0.290	

Charge diff. 5

Class 5: Ordered double perovskites or elpasolites

Rock Salt

No.	compound	Δ IR	comments
1.	$ALaMgIrO_6$	0.015	A = Ca, Sr, Ba
2.	$ALaMgMoO_6$	0.110	A = Ca, Sr, Ba
3.	$ALaMnMoO_6$	0.220	A = Ca, Sr, Ba
4.	$BaLaCoRuO_6$	0.180	
5.	$BaLaFeRuO_6$	0.200	
6.	$BaLaMgRuO_6$	0.155	
7.	$BaLaNiRuO_6$	0.125	
8.	$BaLaZnRuO_6$	0.175	
9.	$SrLaCoNbO_6$	0.105	
10.	$SrLaCoSbO_6$	0.145	
11.	$SrLaCoTaO_6$	0.105	
12.	$SrLaCuNbO_6$	0.040	
13.	$SrLaCuSbO_6$	0.000	
14.	$SrLaCuTaO_6$	0.040	
15.	$SrLaFeTaO_6$	0.140	
16.	$SrLaMgWO_6$	0.100	
17.	$SrLaMnWO_6$	0.210	
18.	$SrLaNiNbO_6$	0.050	
19.	$SrLaNiSbO_6$	0.090	
20.	$SrLaNiTaO_6$	0.050	

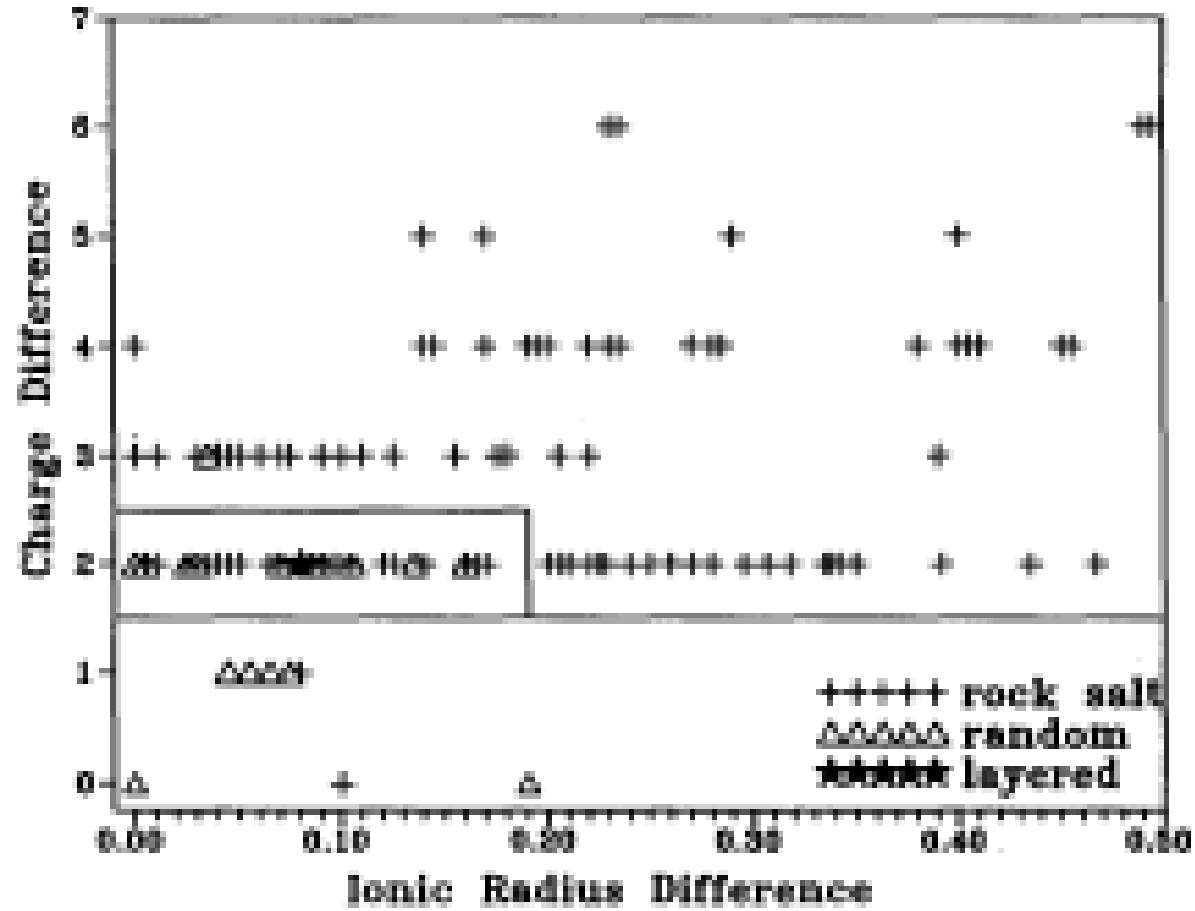
Charge diff. 3

Rock Salt

No.	compound	Δ IR	comments
1.	A_2CoWO_6	0.125	A = Sr, Ba
2.	A_2CuWO_6	0.000	A = Sr, Ba
3.	A_2FeWO_6	0.270	A = Sr, Ba
4.	A_2NiWO_6	0.070	A = Sr, Ba
5.	A_2ZnWO_6	0.120	A = Sr, Ba
6.	Ba_2BaOsO_6	0.800	
7.	Ba_2BaUO_6	0.620	
8.	Ba_2CaMoO_6	0.410	
9.	Ba_2CaOsO_6	0.455	
10.	Ba_2CaReO_6	0.450	
11.	Ba_2CaUO_6	0.270	
12.	Ba_2CaWO_6	0.380	
13.	Ba_2CdOsO_6	0.405	
14.	Ba_2CdReO_6	0.400	
15.	Ba_2CdUO_6	0.220	
16.	Ba_2CoReO_6	0.195	
17.	Ba_2CoUO_6	0.015	
18.	Ba_2CuUO_6	0.010	
19.	Ba_2FeReO_6	0.230	
20.	Ba_2MgReO_6	0.170	
21.	Ba_2MgUO_6	0.010	
22.	Ba_2MgWO_6	0.100	
23.	Ba_2MnReO_6	0.280	

Charge diff. 4

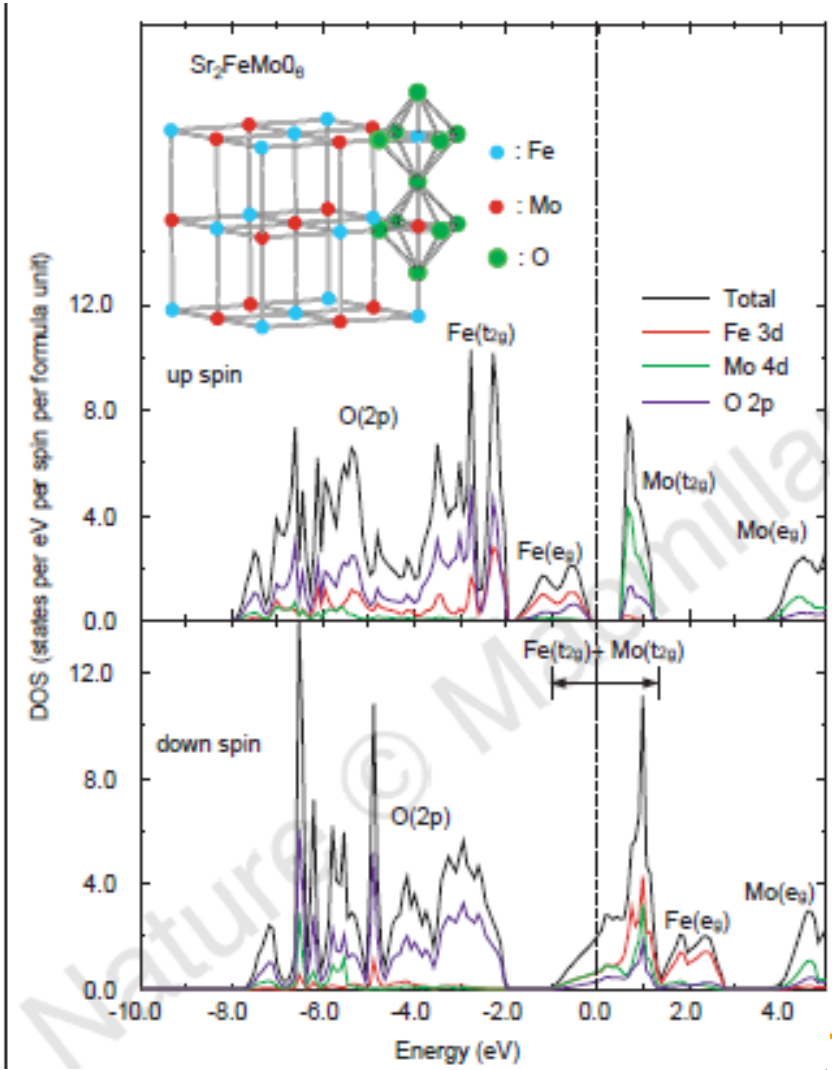
Class 5: Ordered double perovskites or elpasolites

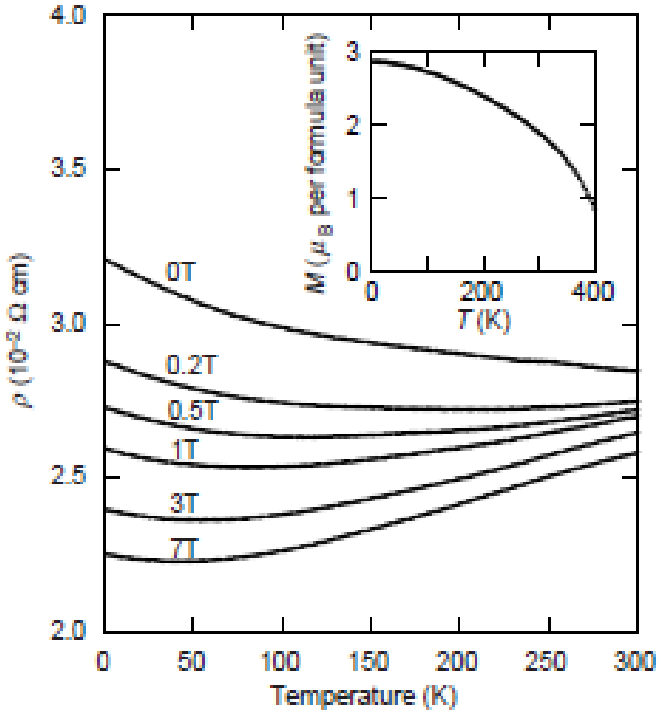


Random, rock-salt and layered structures

Class 5: Elpasolite applications: 1. High-T_c metallic ferromagnet, CMR: Sr_2FeMoO_6

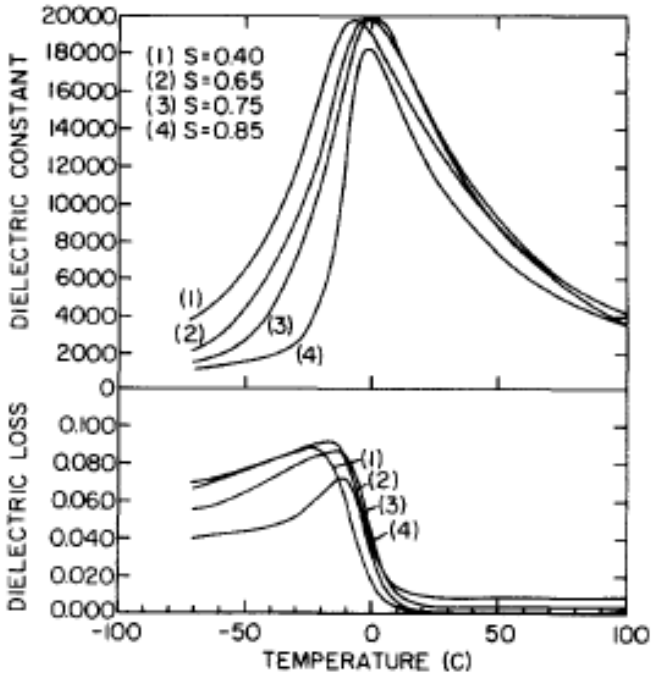
Kobayashi et al. Nature 395 (1998) 677 LINK



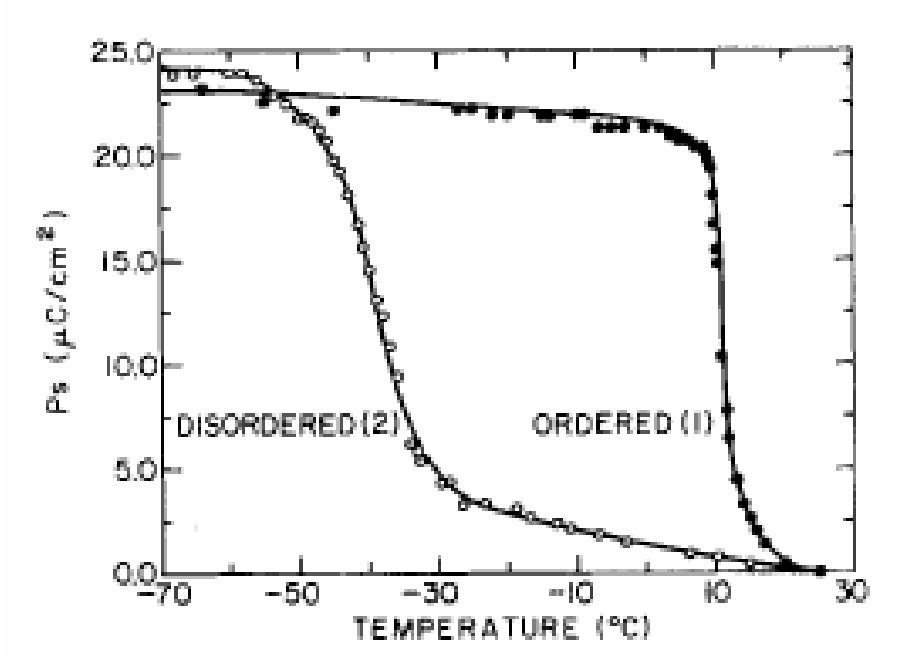


Ferromagnet below 420 K.

Class 5: Elpasolite applications: 2. Relaxor ferroelectrics, Pb_2ScTaO_6 etc.

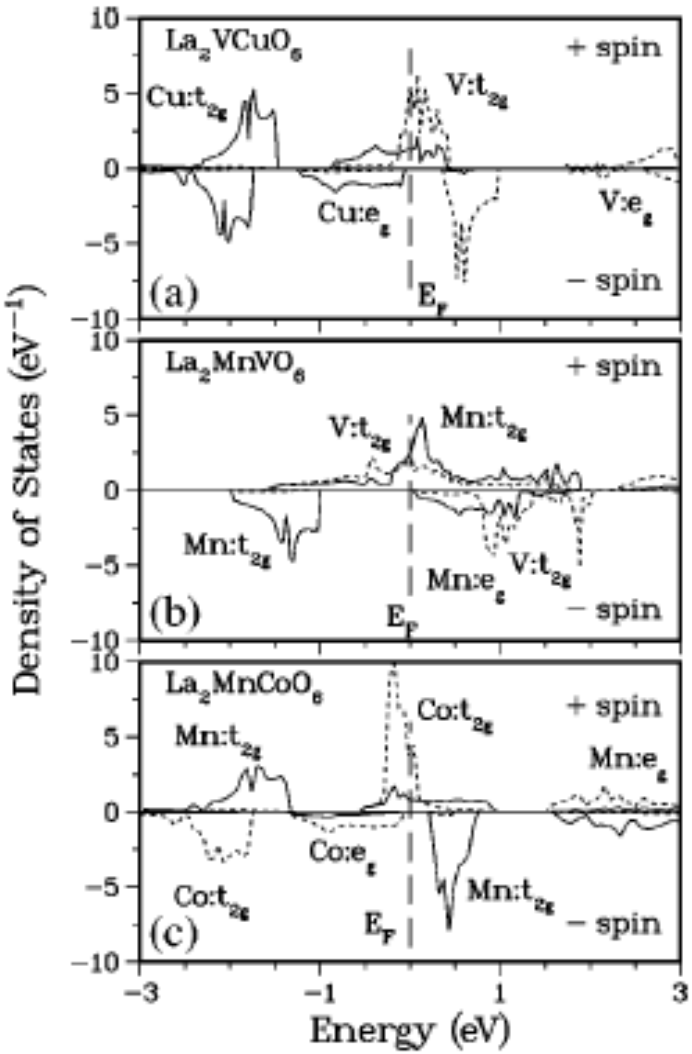


N. Setter and L. E. Cross, J. Appl. Phys. 51 (1980) 4356. LINK



Class 5: Elpasolite applications: 3. Half-metallic antiferromagnets

W. E. Pickett, Phys. Rev. Lett. 57 (1998) 10618 LINK



A nonmagnetic metal whose electrical conduction is 100% spin polarized seems like an oxymoron. However, this is only one of the peculiar properties of the unusual phase yclept half-metallic antiferromagnet by van Leuken and de Groot.