Novel Copper Fluoride Analogs of Cuprates

Supporting Materials

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Table 1: Structure of $C2/m$-Cu_2F_5 optimized using DFT (left) and DFT+U (U=8 eV, J=0.9 eV) (right).

Lattice	Atoms	x	y	z
a = 5.16	Cu1	0.50	0.50	0.50
b = 5.16	Cu2	0.00	0.00	0.50
c = 3.78	F1	0.19	0.19	0.27
α = 104.80	F2	0.80	0.80	0.72
β = 104.80	F3	0.23	0.76	0.50
γ = 95.10	F4	0.76	0.23	0.50
V = 93.1 Å^3	F5	0.50	0.50	0.00

Lattice	Atoms	x	y	z
a = 5.0165	Cu1	0.50	0.50	0.50
b = 5.0165	Cu2	0.00	0.00	0.50
c = 3.6715	F1	0.80	0.80	0.75
α = 106.44	F2	0.19	0.19	0.24
β = 106.44	F3	0.24	0.75	0.50
γ = 95.07	F4	0.75	0.24	0.50
V = 83.62 Å^3	F5	0.50	0.50	0.00

Table 2: Structure of $R\bar{3}c$-CuF_3 optimized using DFT (left) and DFT+U (U=8 eV, J=0.9 eV) (right).

Lattice	Atoms	x	y	z
a = 5.30	Cu1	0.50	0.50	0.50
b = 5.30	Cu2	0.00	0.00	0.00
c = 5.30	F1	0.65	0.84	0.25
α = 58.2	F2	0.34	0.15	0.75
β = 58.2	F3	0.25	0.65	0.84
γ = 58.2	F4	0.15	0.75	0.34
V = 100.9 Å^3	F5	0.84	0.25	0.65
	F6	0.75	0.34	0.15

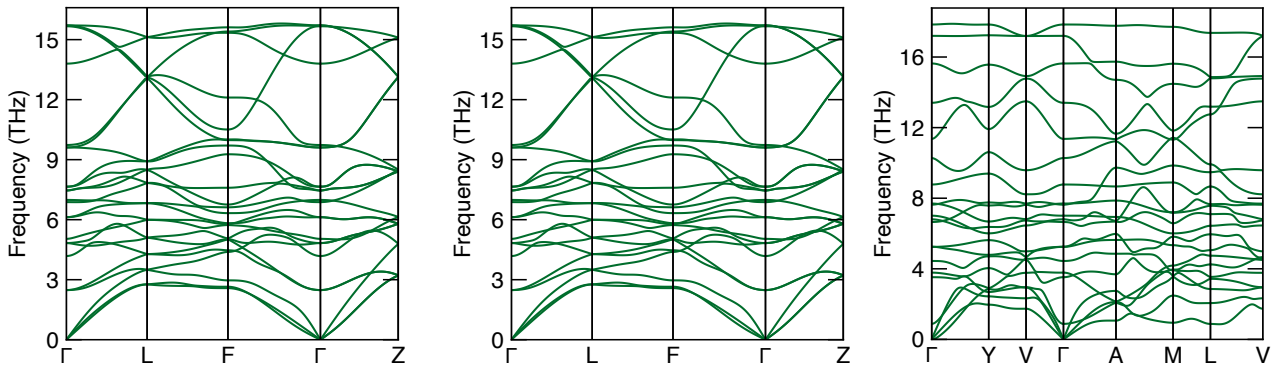
Lattice	Atoms	x	y	z
a = 5.0806	Cu1	0.50	0.50	0.50
b = 5.0806	Cu2	0.00	0.00	0.00
c = 5.0806	F1	0.75	0.10	0.39
α = 56.65°	F2	0.34	0.15	0.75
β = 56.65°	F3	0.10	0.39	0.75
γ = 56.65°	F4	0.60	0.25	0.89
V = 85.55 Å^3	F5	0.39	0.75	0.10
	F6	0.89	0.60	0.25

Table 3: Total energy in eV per formula unit obtained by DFT.

DFT	$R\bar{3}c$-CuF_3	$Pnma$-CuF_3	Cu_2F_5	$Im\bar{3}m$-$K_{0.75}CuF_3$
Spin-unpolarized	-14.6376	-14.6207	-26.7237	-155.4913
Spin-polarized	-14.7456	-14.7259	-26.8182	-155.4913

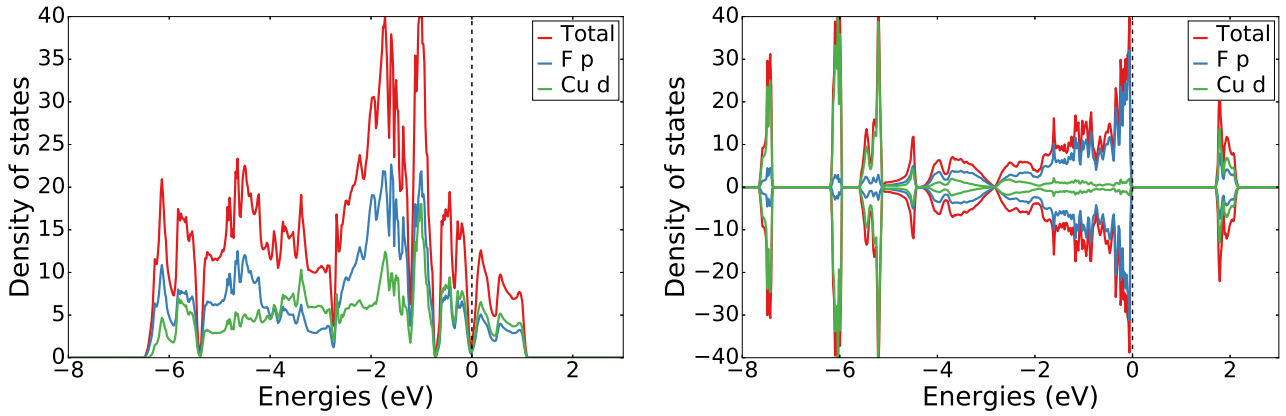
Table 4: Total energy in eV per formula unit obtained by DFT+U (U=8 eV, J=0.9 eV).

Magnetic order	$Bmab$-La_2CuO_4	Cu_2F_5	$Pnma$-CuF_3	$R\bar{3}c$-CuF_3
FM	-49.4917	-22.8729	-12.5685	-12.2429
AFM	-49.7076	-23.2520	-12.6731	-12.6993



(a) (b) (c)

Figure 1: Phonon dispersion curves of (a) *Pnma*-CuF_3, (b) $R\bar{3}c$-CuF_3, and (c) $C2/m$-Cu_2F_5. We used supercell constructed from the primitive unit cell: $3\times3\times3$ for $R\bar{3}c$-CuF_3 and $C2/m$-Cu_2F_5, and $2\times2\times3$ for *Pnma*-CuF_3.



(a) (b)

Figure 2: Density of states of *Pnma*-CuF_3 obtained using (a) DFT and (b) DFT+U (U=8 eV, J=0.9 eV).

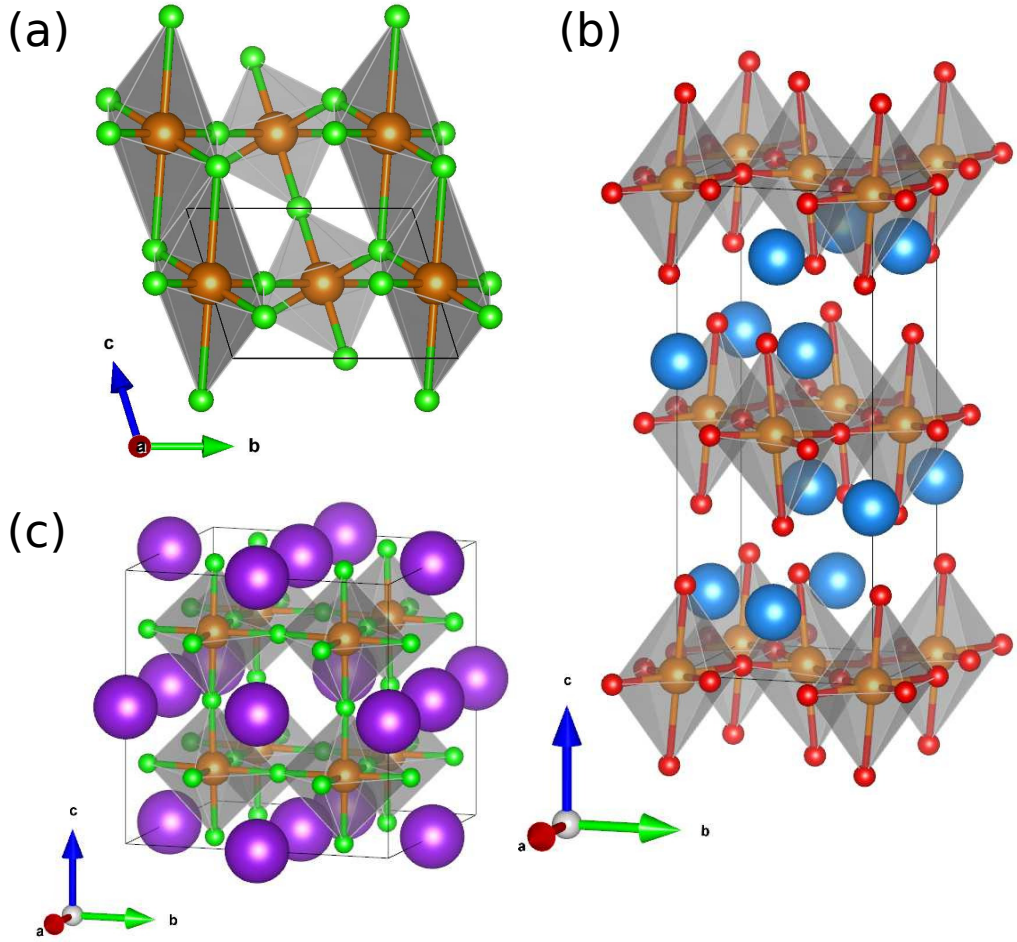


Figure 3: (color online) Schematic representation of the crystal structures: (a) $C2/m$-Cu_2F_5,(b) $Pmab$-La_2CuO_4, and (c) $Im\bar{3}m$-$K_{0.75}CuF_3$. The Cu atom is brown, F is green, O is red, K is purple, and La is blue.