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Electronic structures for skutterudite-related crystals

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For about three decades, it has been known that $Sc(OH)_3$, WAl_{12} and $CaCu_3Mn_4O_{12}$ crystallize in filled skutterudite-related structures.[1,2]

$CaCu_3Mn_4O_{12}$ is one of a large family of $AA'_3M_4O_{12}$ compounds (A = Na, Ca, Sr, rare earth, Th or U; A' = Cu or Mn; M = Ti, Ta, Mn, Fe, Ru or Sb).[17, 25] $CaCu_3Ti_4O_{12}$ has attracted much interest because its dielectric constant approaches 10^5 at low frequencies.[14, 17] In this work, we have carried out FLAPW electronic band structure calculations for $LaCu_3Ru_4O_{12}$ and $CaCu_3Mn_4O_{12}$.

We have also carried out band structure calculations for WAl_{12} type $MnAl_{12}$ and $MoAl_{12}$.

Table 1: Compounds with some structures topologically related to filled skutterudite RT_4X_{12}. The space group is $Im\bar{3}$, T_h^5, #204.

Multiplicity,		Site	Compounds			
Wyckoff letter	Coordinates	symmetry	RT_4X_{12}	$Sc(OH)_3$	WAl_{12}	$CaCu_3Mn_4O_{12}$
2a	(0,0,0)	T_h	R	–	W	Ca
6b	(0,1/2,1/2)	D_{2h}	–	–	–	Cu
8c	(1/4,1/4,1/4)	S_6	T	Sc	–	Mn
12d	(x,0,0)	C_{2v}	–	–	–	–
12e	(x,0,1/2)	C_{2v}	–	–	–	–
16f	(x, x, x)	C_3	–	–	–	–
24g	($0, y, z$)	C_{1h}	X	OH	Al	O
48h	(x, y, z)	C_1	–	–	–	–
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