Table I. Interatomic potentials for $CaCuO_2Cl_2$

(a) Short range: $V(r) = A\exp(-r/\rho) - C/r^6$

Interaction	A(eV)	ρ(Å)	C(eVÅ^6)
$Cu^{2+} \ldots O^{2-}$	4011.0795	0.239415	0.09
$Cu^{2+} \ldots Cl^-$	16091.071341	0.22742	0.58
$O^{2-} \ldots O^{2-}$	22764.3	0.149	63.08
$Cl^- \ldots Cl^-$	27017.414822	0.249784	100.0
$O^{2-} \ldots Cl^-$	342.87	0.28696	0.0
$Ca^{2+} \ldots O^{2-}$	1090.4	0.3437	0.0
$Ca^{2+} \ldots Cl^-$	2302.0	0.3402	0.0

(b) Shell model: $\alpha = Y^2/k$

Species	Y(eV)	k(eVÅ^{-2})
Ca^{2+}	3.135	110.2
Cu^{2+}	2.0	99999.0
Cl^-	-2.519	29.38
O^{2-}	-2.389	42.0