Double Perovskite Crystal Structure

Sr_2FeMoO_6

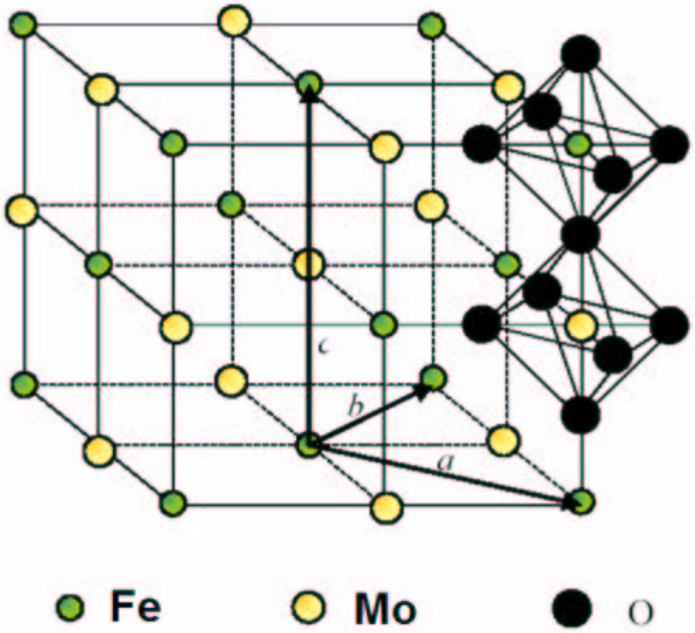
Sr	$5s^2$	2+ (4+)
Fe	$3d^6\ 4s^2 \rightarrow 3d^5$	3+
Mo	$4d^5 5s^1 \rightarrow 4d^1$	5+
O	$2s^2\ 2p^4 \rightarrow 2s^2\ 2p^6$	2- (12-)

Magnetic active orbitals, Fe (5/2)

Distance Fe−Fe is larger than 5.5Å no direct interaction

Electrons live in Mo (1 electron per Fe)

Two interpenetrating FCC Sublattices (Fe and Mo)



Ideal double perovskite structure

$Sr \rightarrow Sr_{1-x}La_x$ **1+x** electron per Fe (trivalent)

$Sr \rightarrow Sr_{1-x}K_x$ **1-x** electron per Fe (monovalent)

Mo → Re **2** electron per Fe **(Re: $5d^5 6s^2$)**

$0.5 < x < 1.5$