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First-principles DFT study of electronic and magnetic properties of Ca_2FeMnO_6: A layered double-perovskite.

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Abstract: The double perovskites ($A_2BB'O_6$) which usually formrock-salt ordered structure are quite promising due to their intriguing properties. Surprisingly,Ca_2FeMnO_6(CFMO, Fig. 1) adoptsan unusual two-dimensional layered ordering of B-site cations[1], hence, facilitating a charge disproportionation (CD) in the Fe-layer[2].We employ first-principles DFT calculations to investigate the role of spin, charge and lattice degrees of freedom in the system, and their mutual coupling, in the observed CD and metal-insulator transitions in CFMO.

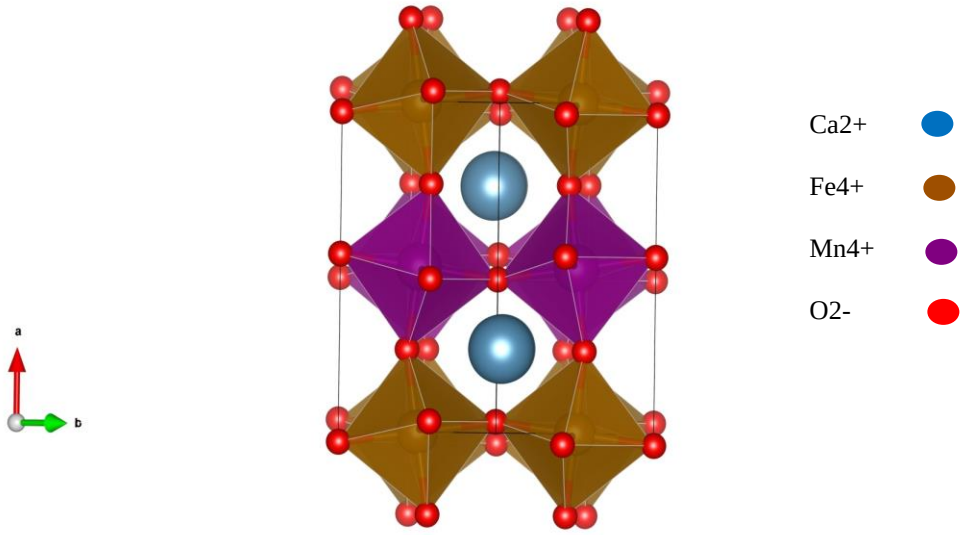

Fig. 1: Structure of Ca_2FeMnO_6

Monoclinic ($P2_1/c$)

a= 7.4951 A^0 ,b = 5.2960 A^0, c = 5.3174 A^0 , β= 89.99

References

1. Hosaka, Y.; Ichikawa, N.; Saito, T.; Manuel, P.; Khalyavin, D.; Attfield, J.; Shimakawa, Y. *Journal of the American Chemical Society* 2015, *137*.

2.Yang, K.; Khomskii, D.; Wu, H. *Physical Review B* 2018, *98*