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Size control of Magnetism, Charge and Orbital Order in Half-Doped Manganite, $La_{0.5}Ca_{0.5}MnO_3$[1] TANUSRI SAHA-DASGUPTA, S.N.Bose National Centre for Basic Sciences, HENA DAS, Cornell University, G. SANGIOVANNI, A. VALLI, K. HELD, Institute for Solid State Physics, Vienna University of Technology, 1040 Wien, Austria — Motivated by recent experimental results, we study the effect of size reduction on half-doped manganite, $La_{0.5}Ca_{0.5}MnO_3$, using the combination of density functional theory (DFT) and dynamical mean field theory (DMFT). We find that upon size reduction, the charge-ordered antiferromagnetic phase, observed in bulk, to be destabilized, giving rise to the stability of a ferromagnetic metallic state. Our theoretical results, carried out on defect-free nanocluster in isolation, establish the structural changes that follow upon size reduction to be responsible for this. Our study further points out the effect of size reduction to be distinctively different from application of hydrostatic pressure. Interestingly, our DFT+DMFT study, additionally, reports the correlation-driven stability of charge-orbitally ordered state in bulk $La_{0.5}Ca_{0.5}MnO_3$, even in absence of long range magnetic order.

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