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Novel electronic and magnetic properties of a new class of cupper oxides XIAO HU, XIANGANG WAN, MASANORI KOHNO, National Institute for Materials Science, Tsukuba 305-0047, Japan — Cuprates have not been considered seriously as candidate of useful magnetic material since the known ferromagnetic cuprates show quite low T_c. The recently reported cuprate Sr_8 $CaRe_3Cu_4O_{24}$, a Mott insulator with perovskite structure, exhibits surprisingly macroscopic magnetization up to $T_c = 440K$. Doing LSDA+U calculations, we reveal theoretically [X.-G. Wan, M. Kohno, and X. Hu, Phys. Rev. Lett. vol. 94, 087205 (2005).] that an orbital order appears in Cu atoms which results in a ferrimagnetic ground state, and that the pdσ bonds are responsible to the strong super exchange interactions and thus the high T_c. We propose a spin model and perform quantum Monte Carlo simulations, with which we can reproduce accurately the observed magnetization curve including the critical point T_c. Moreover, a half-metal (HM), which behaves as metal for one spin channel and insulator for the opposite, is predicted when replacing Re with W or Mo [X.-G. Wan, M. Kohno, and X. Hu, Phys. Rev. Lett. vol. 95, 146602 (2005)]. Hole doping into the material will also result in HM, with the net magnetic moment changing from negative to positive upon tuning the doping rate. Therefore, an antiferromagnetic HM, a material which has yet been found so far, may be achieved where net magnetization disappears.

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