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Magnetic properties of $Sr_8CaRe_3Cu_4O_{24}$ MASANORI KOHNO, XIANGANG WAN, XIAO HU, Computational Materials Science Center, National Institute for Materials Science, Tsukuba 305-0047, Japan — Magnetic properties of $Sr_8CaRe_3Cu_4O_{24}$ are investigated by numerical simulations. This material has anomalously high Curie-temperature (T_c=440K) among ferromagnetic cuprates. The magnetic effective model of this compound is derived based on the LSDA+U result as a spin-alternating Heisenberg model in three dimensions. We apply quantum Monte Carlo methods (the loop algorithm and the directed-loop algorithm) to the effective model. The temperature-dependence of the magnetization is consistent with experimental results. The effective coupling constant J is estimated as about 700K. We further predict magnetic properties of this compound through investigation of the effective model. Numerical results of susceptibilities near the transition point indicate that the transition is second order and belongs to the universality class of the three-dimensional Heisenberg model. Behaviors of the specific heat at finite temperatures and the magnetization process in the low-temperature regime are also investigated. Some of the numerical results on the effective model may be accessible experimentally.

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