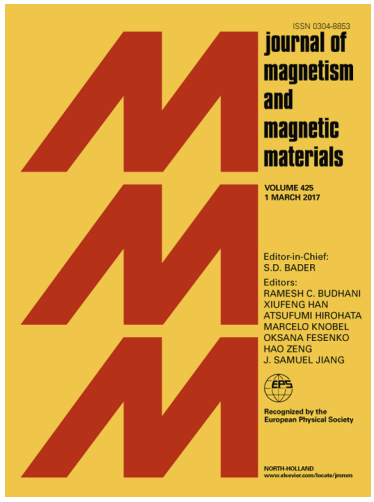

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Investigation by Monte Carlo simulation of substitution doping in the Double Perovskite $Sr_2CrRe_{1-x}W_xO_6$

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Abstract:

Re-substitution doping by W has been investigated in the Double Perovskite (DP) $Sr_2CrRe_{1-x}W_xO_6$ for x ranging from 10 to 90% by using a Monte Carlo Simulation (MCS) in the framework of Ising model. Exchange couplings used in the simulation have been approximated in previous work for experimental Curie temperatures (T_C). Doping effect on: partial and total magnetization, magnetic susceptibility, internal energy, specific heat, and Curie temperature has been studied. A sharp drop of partial magnetizations at 40 % of W-concentration has been noticed at the magnetic transition. Apparition of a non-monotonic behavior of the total magnetization at 20% of W-concentration. Effect of doping on the stability of the compound has been emphasized. A quasilinear decrease of T_C has been observed by increasing the concentration percentage of substitution doping by W.

***Keywords*:** Double Perovskite; Super exchange; Double exchange; Internal energy per site; Monte Carlo Simulation.

1- Introduction:

Magnetic materials with a perovskite structure are transition-metal oxides that attract enormous research interest thanks to their wide variety of remarkable properties like: giant magnetoresistance “GMR” [1, 2], half-metallicity [3], metal-insulator transition [4, 5], multiferroicity [6], high ordering temperature [7]. DPs ($A_2BB'O_6$, A = alkaline earth metals and B-B’ = transition metals) are serious candidates for application in various areas going from spintronics to vehicle batteries, sensors, displays, lasers and much more. Sr_2CrWO_6 and Sr_2CrReO_6 are DPs belonging to this class of materials with half-metallic ferromagnetic behavior above room temperature and high T_C which is important in the area of spintronics. In addition, both materials present high spin polarization which is essential for application in spintronic applications. Sr_2CrWO_6 has been reported to crystallize in a cubic cell (space group symmetry: $Fm\bar{3}m$) with $a = 7.832$Å. $N_v = 4$ is its total number of valence electrons supplied by Cr and W. Its calculated magnetic structure indicates that it’s a half-metallic ferrimagnet. $M_{\mathrm{tot}}^{\mathrm{calc}} = 2.0\mu_B\ /f.u.$ is its total