Monte Carlo calculations of Curie temperature of $Y_{1-x}Gd_x(Fe_{1-y}Co_y)_2$ pseudobinary system

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The $Y_{1-x}Gd_x(Fe_{1-y}Co_y)_2$ system belongs to Laves phases [1,2], which are binary close-packed structures with the chemical composition AB_2. Our main result is the dependence of the Curie temperature on the Gd and Co concentrations of the $Y_{1-x}Gd_x(Fe_{1-y}Co_y)_2$ system, obtained by fashioning the Heisenberg model Hamiltonian of the mentioned system with Monte Carlo simulations using parameters from the first-principles calculations. Furthermore, we investigate the dependence of exchange integrals on inter-atomic distance and study the behavior of total and partial magnetic moments as calculated from the first principles. For the $Y_{1-x}Gd_xFe_2$ system we reproduced the linear dependence of T_C on Gd concentration x and for the $Y(Fe_{1-y}Co_y)_2$ and $Gd(Fe_{1-y}Co_y)_2$ we reproduced the characteristic Slater-Pauling-like dependence of T_C on Co concentration y.

References:

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We acknowledge financial support from the Foundation for Polish Science grant HOMING. The HOMING program is cofinanced by the European Union under the European Regional Development Fund. MW acknowledges the financial support of the National Science Centre Poland under the decision DEC-2018/30/E/ST3/00267.