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Electronic Structure, Chemical Bonding and Magnetic Properties in the Intermetallic Series $Sc_2Fe(Ru_{1-x}Rh_x)_5B_2$ from First Principles¹ GERMAN SAMOLYUK, Department of Chemistry, Iowa State University, Ames, IA, BONIFACE FOKWA, RICHARD DRONSKOWSKI, Institute of Inorganic Chemistry, RWTH Aachen University, Landoltweg 1, Aachen, Germany, GORDON MILLER, Department of Chemistry, Iowa State University, Ames, IA — Firstprinciples, density-functional studies of the electronic structure, chemical bonding, ground-state magnetic ordering and exchange-interaction parameters have been performed for the entire $Sc_2Fe(Ru_{1-x}Rh_x)_5B_2$ series of magnetic compounds. The results indicate that their magnetic properties depend in an extremely sensitive way on the degree of band filling and bandwidth. Continuous substitution of Ru by Rh changes the ground state from an antiferromagnet to a ferromagnet, as well as increases the effective spin moment caused by filling the bands with five additional electrons per formula unit together with a narrowing of the 4d band. The correlations between the character of the chemical bonding and the resulting exchange couplings are discussed. Trends for the macroscopic ordering temperatures are correctly reproduced.

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