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There is more to d-electrons than Hubbard U and Hund's rule J
HUGO U. R. STRAND, University of Gothenburg, SE-41296 Gothenburg, Sweden, NICOLA LANATÀ, Rutgers University, Piscataway, New Jersey 08856-8019, USA, MATS GRANATH, BO HELLSING, University of Gothenburg, SE-41296 Gothenburg, Sweden — Multi-band Hubbard models including all d-bands are central for the description of many interesting correlated materials, e.g., the Iron based High-T_c materials. In this work we compare two prevailing spin and angular momentum rotationally invariant models for the local dd-interaction, the generalized Kanamori interaction, and the Slater-Condon atomic Coulomb interaction, and establish how the first can be mapped to a very special case of the former. Using the recently developed multi-band Gutzwiller approximation solver, we show that the partial localization of orbital moments in the intermediately correlated regime of the paramagnetic state, is poorly described by the Kanamori model containing only Hubbard and Hund's rule interactions. In fact, for some integer fillings it differs qualitatively compared to the Slater-Condon interaction.

Hugo U. R. Strand
Department of Physics, University of Gothenburg,
SE-41296 Gothenburg, Sweden

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