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Calculation of Multipolar Exchange Interactions in Spin-Orbital Coupled Systems[1] SHU-TING PI, RAVINDRA NANGUNERI, SERGEY SAVRASOV, Dept. of Physics, UC Davis — A new method of computing multipolar exchange interaction in spin-orbit coupled systems is developed using multipolar tensor expansion of the density matrix in LDA+U electronic structure calculation. Within mean-field approximation, exchange constants can be mapped into a series of total energy calculations by pair-flip technique. Application to Uranium dioxide shows an antiferromagnetic superexchange coupling in dipoles but ferromagnetic in quadrupoles which is very different from past studies. Further calculation of spin-lattice interaction indicates it is of the same order with superexchange and characterizes the overall behavior of quadrupolar part as a competition between them.

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