To the origin of strong electron correlations in 3d/4f/5f compounds

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Strong correlations are charged to be a reason of unability of the first principles studies based on the local density approximation (LDA) to describe the insulating ground state of 3d/4f oxides causing a need to extend it by using U term (LDA+U), GGA or DMFT approaches. Also strong correlations are regarded to be a reason for heavy-fermion phenomena at low temperatures in cerium, ytterbium or actinide intermetallics. According to the Quantum Atomistic Solid-State Theory (QUASST) the strong correlations are predominantly related with the charge transfer during the formation of a compound and with the intra-atomic correlations leading to the formation of the strongly-correlated atomic like systems $3d^n$, $4f^n$ or $5f^n$ with n being an integer number. Such quantum-mechanical object experiences in a crystal the multipolar charge potentials described customarily as the crystal field. We consistently described a monoxide NiO, reconciling its insulating ground state and a strong magnetism related to eight $3d$ electrons in the incomplete $3d$ shell, and intermetallic UPd_2Al_3 for which neutrons confirm a low-energy structure being a fingerprint of the strongly-correlated $5f^3$ configuration. Recently strongly-correlated $4f^{13}$ systems have been revealed in heavy-fermion metal $YbRh_2Si_2$ at 1.5 K, 15 times lower than the Kondo temperature. We claim that the crystal-field interactions should be evaluated the first for any meaningful description of magnetic and electronic properties both ionic and intermetallic compounds. The many-electron crystal-field approach has inherently incorporated strong-electron correlations.

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13.4 cm

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