Crystal field and orbital magnetism as a Polish contribution to the world physics - Quantum Atomistic Solid State Theory - Magnetic Phase Transitions described at the atomic scale (NiO, UPd_2Al_3)

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Theoretical description of magnetic, electronic and spectroscopic properties as well as the electronic structure of compounds containing transition-metal atoms is still a subject of strong debate within the modern solid-state physics community. Even magnetic and insulating properties of monoxides FeO, CoO and NiO are not yet well theoretically understood, despite a fact that these compounds form the simple crystallographic structure (NaCl) and the simple antiferromagnetism (T_N of 191 K, 291 and 525 K, respectively). In compounds like $YbRh_2Si_2$ or UPd_2Al_3, despite of the heavy-fermion and metallic behaviour, localized states have been recently detected.

We understand the scientific work as searching for the scientific truth which is reached through a consensus within the scientific community. Thus, we turn to the Polish community to work for the consensus about the importance of the localized magnetism as an opposition to the widely popular band picture. The developed Quantum Atomistic Solid-State Theory (QUASST) proposes to start description of $3d/4f/5f$ compounds from the description of the $3d/4f/5f$ atoms/ions forming a solid [1].

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We would like to propose, making use of a large solid-state physics potential in Poland, the crystal field and the orbital magnetism to be a Polish contribution to the world physics. It is desired to openly discuss a most general problem like there is, or not, a crystal field in $3d/4f/5f$ transition-metal compounds, the origin of the magnetocrystalline anisotropy (single-ion or others) or the importance of the orbital magnetism as contrasting commonly used quenching of the orbital moment in $3d$ compounds. The application of QUASST will be illustrated by presentation of our atomic-scale description of NiO [2], the simplest and the widely discussed Mott-insulator compound, and in heavy-fermion metallic superconductor UPd_2Al_3 and in conventional $ErNi_5$.

A quite long list of compounds described within QUASST will be presented: monoxides FeO, CoO and NiO [2], perovskites like $YTiO_3$ [3], $LaMnO_3$ and $LaCoO_3$ [4]. All of these compounds are known as Mott insulators. In $YTiO_3$ Ti^{3+} ion has only one d electron it makes this system examplary one for study of properties the Ti^{3+} ion in the distorted octahedral crystal field in the presence oft he spin-orbit coupling [3]. $YTiO_3$ is ferromagnet with T_C of 30 K. We study the electronic structure both in the paramagnetic state and the ferromagnetic state tracing its change at T_C. The magnetic phase transition is visible, in particular, in the temperature dependence of the specific heat producing a λ-type of peak at T_C. The magnetic transition, related with breaking of the time-reversal symmetry, is seen in the shape of the eigenfunction.

Our approach to $3d$ compounds combines the solid-state physics with the atomic physics and reveals the importance of the orbital magnetism in description of $3d$-atom containing compounds. The many-electron crystal-field approach takes into account strong electron correlations.

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