We have found atomic-scale description of NiO!

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We have solved an old and fundamental problem of NiO - why it is insulator having incomplete 3d shell. Our solution is in agreement with a Sir Mott's suggestion (for it NiO is regarded as the exemplary Mott insulator) that the insulating ground state is caused by strong electron correlations. However, the nature of strong correlations was discussed by last 50 years and is still a subject of a hot debate in most prestigious physical journals. According to the Quantum Atomistic Solid-State Theory (QUASST) the strong correlations are predominantly related with the charge transfer during the formation of the compound and with the intra-atomic correlations. We have proved that the many-electron crystal-field approach is an approach with inherently incorporated strong electron correlations. We provide consistent description of monoxide NiO, which reconciles its insulating ground state and a strong magnetism related to $3d$ electrons, in a number of eight, in the incomplete $3d$ shell. We have evaluated the real multipole potential, in the atomic scale, in contrary to generally introduced pseudopotentials. For the low-energy electronic structure and for the formation of the magnetically-ordered state the spin-orbit coupling is fundamentally important. We have reproduced values of the magnetic moment and its direction in the $NaCl$ structure. We have found that small lattice distortions determine the direction of the magnetic moment. We have revealed a quite substantial orbital magnetic moment, of 0.54 μ_B.

9.7 cm

13.4 cm

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