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LDA+ U applied to oxide and nitride wide-band-gap semiconductors¹

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Nitride and oxide semiconductors have important technological applications, but the theoretical understanding of their properties is hampered by the shortcomings of density functional theory (DFT) in the local density approximation (LDA). In particular, DFT-LDA underestimates the binding energy of the semicore d states, leading to poor descriptions of quantities such as band offsets and deformation potentials. In this work we calculate the electronic and structural properties of wurtzite MgO, ZnO, and CdO, and discuss their similarities and dissimilarities with the corresponding nitrides AlN, GaN, and InN. We treat the semicore d states of Zn, Cd, Ga, and In explicitly as valence states in a pseudopotential framework, and improve the description of electron-electron interactions in these narrow bands by including an on-site Coulomb interaction through the LDA+ U method. We propose a novel approach to calculate the parameter U , based on first-principles calculations for atoms. The approach is general and could be extended to other semiconductors and insulators where semicore d states play a fundamental role in the description of electronic and structural properties. The LDA+ U approach systematically improves the LDA band gap by indirectly acting on both the valence-band maximum and conduction-band minimum. We investigate the effects of the on-site Coulomb interaction on lattice parameters, band structure, absolute deformation potentials, and band lineups. Finally we discuss how results based on LDA and LDA+ U can be used to calculate defect transition levels and formation energies that can be directly compared with experiment.

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