Optical Absorption Spectra and Dynamic Jahn-Teller Effect of V^{2+} Ions in ZnSe

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The Hamiltonian matrices for $3d^3$ ions in a cubic crystal field are introduced, based on a molecular orbital model, including the electronic Coulomb and tetrahedral crystal-field interactions and the spin-orbit coupling. The optical absorption spectra of V^{2+} ions in ZnSe are studied. Moreover, the various additional levels found close to 5680 cm^{-1} are considered. These levels are assumed to result from the dynamic Jahn-Teller splitting within the excitation levels $^2T_2$ and $^2T_1$ in ZnSe:V^{2+}. The good agreement between the present results and the experimental observations indicates that the contribution of the covalence reduction factors N_E and N_{T_2} and of the Racah parameter A to the optical absorption spectra of V^{2+} ions in ZnSe is important. However, most of the previous theoretical studies of these spectra in ZnSe:V^{2+} have neglected the Racah parameter A, based on the classical crystal-field model. A significant charge-transfer effect found in recent works is confirmed in ZnSe:V^{2+}.

Key words: Semimagnetic Semiconductors; Optical Absorption Spectra;
Dynamic Jahn-Teller Effect; V^{2+} Ions; ZnSe.