The Covalence Effect of the Electron States of ZnSe:Co^{2+}

Jia-Jun Chen[a], Mao-Lu Du[b], and Ti-Xian Zheng[a]

[a] Department of Physics and Electronic Information, China West Normal University, Nanchong 637002, China
[b] Department of Physics, Southwest University for Nationalities, Chengdu 610041, China

Reprint requests to J.-J. C.; E-mail: chenjjnc@nc-public.sc.cninfo.net

Z. Naturforsch. **61a,** 357 – 363 (2006); received April 24, 2006

In the investigation of the optical and magnetic properties of $3d^N$ ion impurities in semiconductors, the contribution of the covalence must be considered. A modified d function (d^*) and two covalent factors associated with the t_2 and e orbitals have been adopted for describing this covalence. We present the contribution of the covalent factors to the energy matrix of the d^{*7} electron and d^{*3} hole system. This suggests that the d^N electron system cannot be explained with the d^{10-N} hole system when the covalence is considered. The calculation of the energy levels by the d^{*7} energy matrix agrees with the experimental finding of ZnSe:Co^{2+}. – PACS numbers: 71.70.Ch, 71.55.Gs

Key words: Ligand-Fields; Covalence Effect; II-VI Semiconductors; Optical Spectra.