The Local Structure Distortion of Chromium-Phosphorus Clusters as Cr\textsuperscript{2+} Impurity in InP Semiconductors

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By diagonalizing the complete energy matrix of a d\textsuperscript{4} configuration ion in tetragonal symmetry, the zero-field-splitting parameters $a$, $D$ and $F$ of InP:Cr\textsuperscript{2+} have been studied. The local structure distortion parameters $\Delta R = 0.08$ Å and $\Delta \theta = 1.01^\circ$ were estimated. They show an expansion distortion around Cr\textsuperscript{2+} in the InP semiconductor. The Jahn-Teller energy $E_{JT}$ is found to be about 413 cm\textsuperscript{-1}, which agrees well with the experiment. – PACS numbers: 75.10.Dg; 76.30.-v

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