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

Xiao-Ming Tan[a], Xiao-Yu Kuang[a,c], Kang-Wei Zhou[b,c,d], Cheng Lu[a], and Qin-Sheng Zhu[a]

[a] Institute of Atomic and Molecular Physics, Sichuan University, Chengdu 610065, China
[b] Department of Physics, Sichuan University, Chengdu 610065, China
[c] International Centre for Materials Physics, Academia Sinica, Shenyang 110016, China
[d] CCAST (World Lab.), P. O. Box 8730, Beijing 100080, China

Reprint requests to X.-Y. K.; E-mail: scu_txm@163.com

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By diagonalizing the complete energy matrix of a d^4 configuration ion in tetragonal symmetry, the zero-field-splitting parameters a, D and F of InP:Cr^{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^{2+} in the InP semiconductor. The Jahn-Teller energy E_{JT} is found to be about 413 cm^{-1}, which agrees well with the experiment. – PACS numbers: 75.10.Dg; 76.30.-v

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