Magnetic interactions of Cr-Cr and Co-Co impurity pairs in ZnO within a band-gap corrected density functional approach

z = z zZZ s

	11	AN D	Z _I s	
Γ . (Γ) ()	0. 3	3.23	3.44	(5.)
· */	0.1	0.4	0.2	(<u></u> .)
• () ()	5.4	.43	.40	()
., -& Z. ()	, 4.	, .0	, . 3 , .5	(<u>s</u> .)
• (⁻³)	4.5	45.02	4.1	(5.)
•// [*]	1. 13	1.5 5	1. 02	(<u></u> .)
	0.3.	0.3	0.3 3	(5.)

Z = Z = (Z = 1) + (Z = 1

 $Z = \begin{bmatrix} z \\ z \end{bmatrix} =$ $Z_{T} = \sum_{i=1}^{N} \sum_{j=1}^{N} \sum_{i=1}^{N} Z_{T} = \sum_{i=1}^{N} \sum_{j=1}^{N} \sum_{i=1}^{N} \sum_{j=1}^{N}$ Z Z Z Z $Z = \frac{1}{2} \left(\frac{1}{2} \right)_{3} Z_{3} \left(\frac{1}{2} \right)_{3} Z_{4} \left(\frac{1}{2} \right)_{4} \left(\frac$ **λ** . **μ**. **λ** Ζ_γΖ₅ ε (+



 $S_{2} = -8 = \frac{\varepsilon(+/0)}{15} = \frac{1}{15} = \frac{$