

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

Abstract: This study investigates the magnetic interactions between Cr-Cr and Co-Co impurity pairs in ZnO using a band-gap corrected density functional theory (DFT) approach. The results show that the magnetic coupling between the impurity pairs is strongly dependent on the distance between them and the nature of the impurity ions. For Cr-Cr pairs, the coupling is generally antiferromagnetic (AFM) at short distances and becomes ferromagnetic (FM) at larger distances. For Co-Co pairs, the coupling is generally ferromagnetic (FM) at short distances and becomes antiferromagnetic (AFM) at larger distances. The band-gap correction significantly affects the calculated magnetic moments and the nature of the magnetic coupling, leading to a more accurate description of the magnetic interactions in ZnO.



$\varepsilon(+/0)$  +1.96  
15  
1  
[1(2)]  
2  
0.1  
72  
1.9  
3.1  $\mu$  ( $10^2$ )  
29

