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First-principles study of structrural and corrected band properties of wurtzite $Zn_{1-x}Cd_xO$ and $Zn_{1-x}Mg_xO$ systems*

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A first-principles method based on density functional theory (DFT), a generalized gradient approximation (GGA), and a projector-augmented wave (PAW) are used to study the structual and band properties of wurtzite $Zn_{1-x}Cd_xO$ and $Zn_{1-x}Mg_xO$ ($0 \leqq x \leqq 1$) ternary alloys. By taking into account all of the possible structures, the band gaps of $Zn_{1-x}Cd_xO$ and $Zn_{1-x}Mg_xO$ alloys are corrected and compared with experimental data.

Keywords: $Zn_{1-x}Cd_xO$ and $Zn_{1-x}Mg_xO$, first-principles, corrected band structure
PACC: 7280E, 7125, 7155M

1. Introduction

ZnO, as a wide and direct band-gap II-VI semiconductor material, is one of the most promising materials for ultraviolet optoelectronic applications due to its wide band gap (3.37eV) and large exciton binding energy (60meV).[1−3] ZnO also has other great potential applications in varistors,[4] solar cell,[5] sensors,[6] nanolaser,[7,8] etc. ZnO and its alloys with MgO and CdO are promising materials for optoelectronic devices that rely on band-gap engineering to provide carrier and optical confinement.[9−11] Doping Cd into ZnO can reduce the band gap while doping Mg can increase the band gap. With modest Cd (Mg) concentration, the ZnMgO (ZnCdO) alloy has a wurtzite structure,[9−12] in spite of the fact that MgO (CdO) occurs in the cubic rocksalt structure. The maximum content of Mg in the wurtzite $Zn_{1-x}Mg_xO$ can reach 0.46[13] or 0.49[14] and a recent experiment has shown that the Mg content increases possibly from 0.44 to 0.66[15] while previous reports suggested that the upper limit of Cd substitution, x, was lower than 0.25, i.e. $x < 0.25$ in wurtzite $Zn_{1-x}Cd_xO$ alloys.[10,16−18] Therefore little research has focused on ZnO/ $Zn_{1-x}Cd_xO$ heterojunctions. Recently, Ishihara *et al* [19] have successfully overcome the limit of cadmium solution in ZnO–CdO alloy systems by remote-plasma-enhanced metal organic chemical vapour deposition.[19] In the $Zn_{1-x}Cd_xO$ films, the Cd content x in the wurtzite structure can increase even up to 0.69, and it is revealed that the $Zn_{1-x}Cd_xO$ alloy films are well suited for optoelectronic applications in an ultraviolet–visible spectral range.

Many *ab initio* calculations of the properties of the parent compounds ZnO, MgO and CdO can be found in the literature.[20−25] But the properties of ternary $Zn_{1-x}Mg_xO$ and $Zn_{1-x}Cd_xO$ alloys have been little studied. Recently, Malashevich and Vanderbilt[26] studied the spontaneous polarization of $Zn_{1-x}Mg_xO$ alloys as a function of their composition by using the density-functional theory (DFT) in the local-density approximation (LDA). Amrani *et al* [27] used the full potential linearized augmented plane wave (FP-LAPW) method to study structural, electronic and thermodynamic parameters of the $Zn_{1-x}Mg_xO$ alloy in the cubic phase. Rozale *et al* [28] studied the ordered structures of $Zn_{1-x}Cd_xO$ alloys within the theoretical framework of order–disorder

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transformation by using the FP-LAPW method. In the present paper, we construct all of the possible structures of wurtzite $Zn_{1-x}Cd_xO$ and $Zn_{1-x}Mg_xO$ alloys and study their structural and band properties at compositions x = 0.00, 0.125, 0.25, 0.375, 0.50, 0.625, 0.75, 0.825 and 1.00, separately.

2. Computational methods

The structures and the electronic bands of wurtzite $Zn_{1-x}Cd_xO$ and $Zn_{1-x}Mg_xO$ ($0 \leqq x \leqq 1$) ternary alloys were investigated by using the projected augmented wave (PAW) method[29−31] as found in the *Vienna Ab initio Simulation Package* (VASP).[32] The calculations were performed by using DFT[33] in the generalized gradient approximation (GGA)[34] of Perdew and Wang (PW91).[35] The PAW method allows the accurate treatment of the first-row element oxygen as well as the Zn 3d, Cd 4d and Mg 2p electrons. We use an energy cutoff of 500 eV for the plane-wave basis set expansion.[23] The Brillouin-zone (BZ) integrations in the electron density, and the total energy were made by using a set of 4×4×4 special points of the Monkhorst–Pack type[36] with a 16-atom supercell which corresponds to a 2×2×1 conventional wurtzite ZnO cell, then 1 to 8 Zn atoms in wurtzite $Zn_{1-x}Cd_xO$ or $Zn_{1-x}Mg_xO$ are replaced with Cd or Mg atoms, respectively. For the computation of the electronic density of states (DOS), we use the tetrahedron method[37] to perform the corresponding BZ integration with 8×8×10 k-space meshes. A first approach to qualitatively reliable band structures is to use the eigenvalues of the Kohn–Sham (KS) equation.[34]

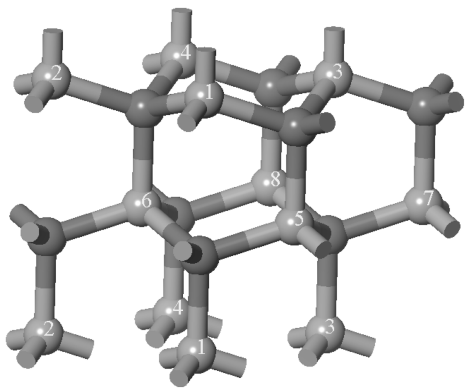


Fig.1. Supercell of ZnO composed of 8 Zn and 8 O atoms, where the numbered atoms are Zn atoms.

In Fig.1 we show the supercell containing 8 Zn and 8 O atoms. The numbered atoms are Zn atoms and the remaining (un-numbered) atoms are O atoms. To study Cd/Mg doped ZnO, we first determine the preferred site of Cd/Mg atoms and how these sites change as the concentration of Cd/Mg increases, and all of the possible structures are listed in Table 1.

Table 1. Relative M (M=Cd, Mg) position of configuration in $Zn_{1-x}M_xO$ alloys. The first column gives the compositions of the supercell, the second column indicates the identity (ID) numbers to be used in the present paper, the third column shows the Zn sites replaced by M, and the last column presents the symmetry of the $Zn_{1-x}M_xO$ alloys. There are three pairs of $Zn_{1-x}M_xO$ alloy configurations that have the same symmetry as those with M concentrations corresponding to ID No. 3-2, 3-3, No. 4-1, 4-4 and 5-2, 5-3, but these three pairs have different closest distances.

system	ID	site occupied by M	symmetry
Zn_8O_8	0-1	null	$P63mc$
$Zn_7M_1O_8$	1-1	8	$P3m1$
$Zn_6M_2O_8$	2-1	1, 8	$P63mc$
	2-2	1, 5	$Cmc21$
	2-3	1, 2	Pm
$Zn_5M_3O_8$	3-1	1, 2, 3	$P3m1$
	3-2	1, 4, 5	Cm
	3-3	1, 2, 5	Cm
$Zn_4M_4O_8$	4-1	1, 2, 3, 4	$P3m1$
	4-2	1, 4, 5, 8	$Pmc21$
	4-3	1, 2, 5, 6	Pmn21
	4-4	1, 2, 3, 5	$P3m1$
	4-5	1, 2, 5, 7	Cc
	4-6	1, 2, 4, 5	Cm
$Zn_3M_5O_8$	5-1	4, 5, 6, 7, 8	$P3m1$
	5-2	2, 3, 6, 7, 8	Cm
	5-3	3, 4, 6, 7, 8	Cm
$Zn_2M_6O_8$	6-1	2, 3, 4, 5, 6, 7,	$P63mc$
	6-2	2, 3, 4, 6, 7, 8	$Cmc21$
	6-3	3, 4, 5, 6, 7, 8	Pm
$Zn_1M_7O_8$	7-1	1, 2, 3, 4, 5, 7, 8	$P3m1$
M_8O_8	8-1	all	$P63mc$

3. Results and discussion

Total energies are calculated first for all configurations. In both $Zn_{1-x}Cd_xO$ and $Zn_{1-x}Mg_xO$ alloys, ID Nos. 2-1, 3-2, 4-2, 5-2 and 6-1 have the low total energies compared with those of relevant configurations which have the same Cd/Mg compositions and are plotted by solid symbols in all figures.

The lattice constants of $Zn_{1-x}Cd_xO$ and $Zn_{1-x}Mg_xO$ alloys are plotted in Figs.2(a) and 2(b), respectively. Figure 2(a) for $Zn_{1-x}Cd_xO$ alloys clearly shows that lattace constants a and c both have a linear

relationship with Cd content especially for configurations with ID Nos. 2-1, 3-2, 4-2, 5-2, 6-1, which is consistent with the linearly increasing fitting line. We can write an equation following Vegard's law:

$$\alpha_{(Zn_{1-x}Cd_xO)} = (1-x)\alpha_{ZnO} + x\alpha_{CdO}, \qquad (1)$$

where α_{ZnO} and α_{CdO} are the equilibrium lattice constants of the binary compounds wurtzite ZnO (3.280 Å, 5.296 Å and $u = 0.380$) and CdO (3.677 Å, 5.812 Å and $u = 0.384$) respectively. $\alpha_{(Zn_{1-x}Cd_xO)}$ is the alloy lattice constant. Meanwhile, the experimental results also show a linear increase with Cd content x increasing up to 0.69.[19]

Figure 2(b) shows that for the $Zn_{1-x}Mg_xO$ alloy, lattice constant c decreases nonlinearly and lattice constant a increases nonlinearly. While the measurements also show that lattice constants a and c both non-linearly change with Mg content,[38] and that Vegard's law does not hold has been also reported both experimentally[39,40] and theoretically.[41–44]

Hence, the lattice constants of the $Zn_{1-x}Mg_xO$ alloy may be fitted to the following expression:

$$\alpha_{(Zn_{1-x}Mg_xO)} = (1-x)\alpha_{ZnO} + x\alpha_{MgO} + x(1-x)b, \quad (2)$$

where α_{ZnO} and α_{MgO} are the equilibrium lattice constants of the binary compounds, $\alpha_{(Zn_{1-x}Mg_xO)}$ is the alloy lattice constant and the quadratic term b is the bowing parameter. In our results, the lattice constants a_{MgO} and c_{MgO} of the binary MgO are 3.306 Å, 5.102 Å ($u = 0.387$) and the coresponding values of bowing parameter b are –0.042 and 0.1, respectively.

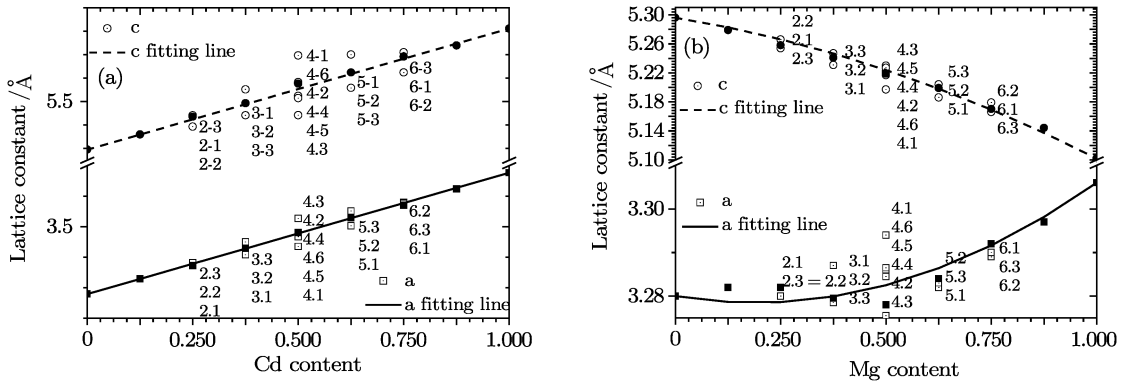


Fig.2. Variations of lattice constants a and c (a) in $Zn_{1-x}Cd_xO$ with Cd content and (b) in $Zn_{1-x}Mg_xO$ alloys with Mg content.

The band structures of $Zn_{1-x}M_xO$ alloys are calculated along some arbitrarily chosen directions in the BZ. Our results show that both the velence band maximum (VBM) and the conduction band mimimum (CBM) are at Γ point, thereby indicating a direct band gap in all of the $Zn_{1-x}M_xO$ alloys. For wurtzite ZnO, CdO and MgO, we obtain direct band gaps of 0.734, –0.0693 and 3.452 eV, respectively. These results are in good agreement with the calculations of wurtzite ZnO, CdO and MgO.[22] For $Zn_{1-x}Cd_xO$ ($0.125 \leqq x \leqq 0.875$) alloys, we obtain a nonlinear decaying band gap from 0.52 to –0.0687 eV. While the experimental results show that the luminescence peak shifted from 3.28 eV of ZnO to 1.73 eV of $Zn_{0.31}Cd_{0.69}O$,[19] which is much larger than our calculation. It is well-known that DFT underestimates the band gaps of semiconductors and insulators, for it gives a lower excited energy. For $Zn_{1-x}Mg_xO$ ($0.125 \leqq x \leqq 0.875$) alloys, we obtain the band gap increasing nonlinearly from 1.021 to 3.131 eV.

The band structures of $Zn_{0.5}Cd_{0.5}O$ and $Zn_{0.5}Mg_{0.5}O$ alloys (No. 4-2) are shown in Figs.3(a) and 3(b), respectively. Both of them show the direct band gap and clearly exhibit that the lower valence bands (VBs) of Cd 3d, Zn 3d and Mg 2p change very slowly and the upper VB of O 2p is flat, which indicates that the values of the effective mass of hole are larger in both $Zn_{1-x}Cd_xO$ and $Zn_{1-x}Mg_xO$ alloys.

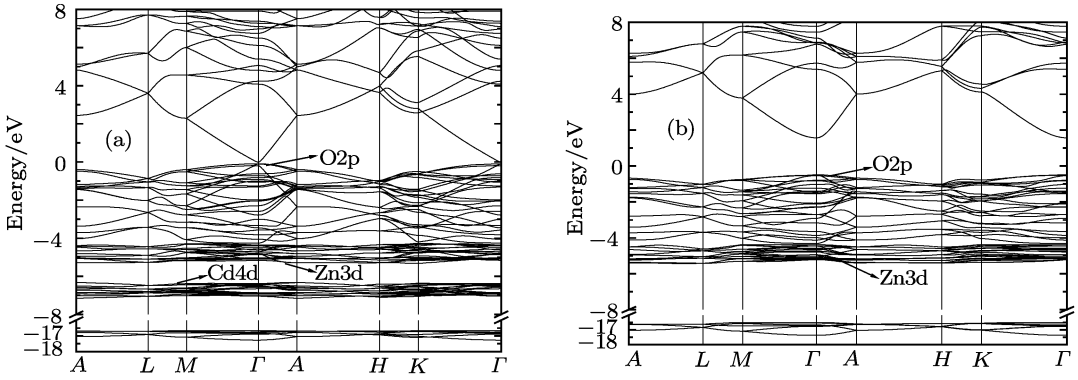


Fig.3. Band structures of (a) $Zn_{0.5}Cd_{0.5}O$ and (b) $Zn_{0.5}Mg_{0.5}$ O alloys (No. 4-2).

The band gaps of $Zn_{1-x}Cd_xO$ and $Zn_{1-x}Mg_xO$ alloys are shown in Fig.4 and compared with the binary fitting curves. According to the virtual-crystal approximation (VCA),[45] the binary equation can be written as follows:

$$E_{g(Zn_{1-x}Cd_xO)} = (1-x)E_{g(ZnO)} + xE_{g(CdO)} + 0.97x(x-1), \quad (3)$$

and

$$E_{g(Zn_{1-x}Mg_xO)} = (1-x)E_{g(ZnO)} + xE_{g(MgO)} + 0.60x(x-1). \quad (4)$$

From Fig.4(a), we find that the curve for the Nos. 2-1, 3-2, 4-2, 5-2, 6-1 in $Zn_{1-x}Cd_xO$ alloys fits well to the nonlinear fitting line, but from Fig.4(b) we can see that the curve for Nos. 2-1, 3-2, 4-2, 5-2, 6-1 in $Zn_{1-x}Mg_xO$ alloys quasi-linearly goes up (the bowing parameter b is only 0.10). While the experiments also show that the band gap has a linear relationship with Mg content in wurtzite $Zn_{1-x}Mg_xO$ alloys.[14,15,46,47] The total energies and the results of structure and band indicate that the configurations corresponding to ID Nos. 2-1, 3-2, 4-2, 5-2, 6-1 are the possible stable structures of both $Zn_{1-x}Cd_xO$ and $Zn_{1-x}Mg_xO$ alloys.

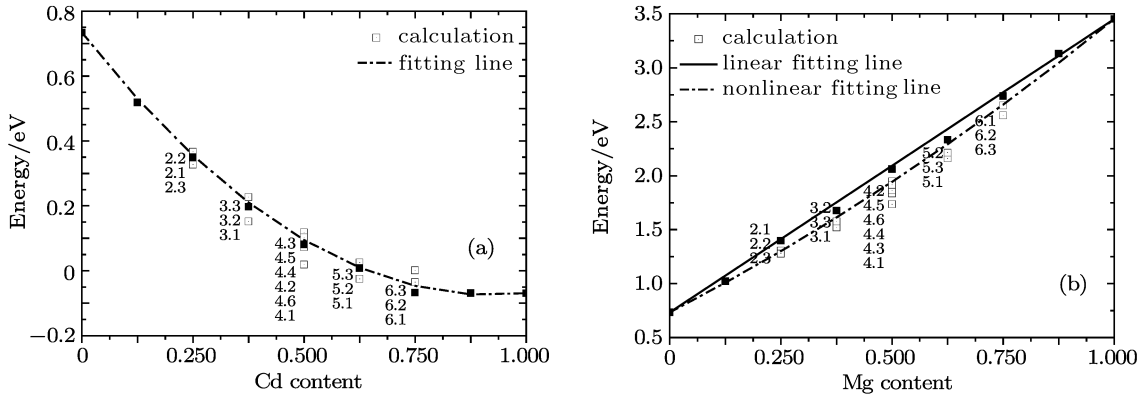


Fig.4. Band gaps of (a) $Zn_{1-x}Cd_xO$ and (b) $Zn_{1-x}Mg_xO$ alloys versus content x.

We also calculate the band structures of rocksalts CdO and MgO and compare the calculations with measurements to simply check the prediction of the band gaps of wurtzite CdO and MgO.[23] The calculated band gaps of rocksalts CdO and MgO are 0.546 and 4.530 eV while the measured values[48] are 2.28 and 7.9 eV, respectively. By adding the band-gap errors in rocksalts CdO and MgO, the predicted band gaps of wurtzite CdO and MgO are 1.665 and 6.822 eV, respectively, which are larger than 0.92 and 6.4 eV given by Janotti *et al* [23] but are in good agreement with the calculation results with the correction

of the CBM (about 1.5 eV) for wurtzite CdO, given by Guerrero-Moreno and Takeuchi.[21] We correct the band gaps of $Zn_{1-x}Cd_xO$ and $Zn_{1-x}Mg_xO$ alloys by performing a linear transform as follows:

$$E_{g(Zn_{1-x}M_xO)_{co}} = E_{g(Zn_{1-x}M_xO)_{ca}} + (1-x) \times (E_{g(ZnO)_{ex}} - E_{g(ZnO)_{ca}}) + x(E_{g(MO)_{pr}} - E_{g(MO)_{ca}}) \quad (M = Cd, Mg), \tag{5}$$

where $E_{g(Zn_{1-x}M_xO)_{co}}$ is the corrected band gap and $E_{g(Zn_{1-x}M_xO)_{ca}}$ is the calculated band gap of $Zn_{1-x}M_xO$ (M=Cd, Mg) alloys, $E_{g(ZnO)_{ex}}$ is the measured band gap and $E_{g(ZnO)_{ca}}$ is the calculated band gap of ZnO, and $E_{g(MO)_{pr}}$ is the predicted band gap and $E_{g(MO)_{ca}}$ is the calculated band gap of MO. The corrected band gaps of $Zn_{1-x}Cd_xO$ and $Zn_{1-x}Mg_xO$ alloys are shown in Figs.5(a) and 5(b), respectively, where, for comparison, their predicted, measured, and cited band gaps, as well as their fitting lines are also given. Figure 5(a) clearly shows that for the corrected band gaps of $Zn_{1-x}Cd_xO$ alloys, their band gap and bowing parameter ($b = 0.95$) are in good agreement with the measurements in Ref.[49], and their variations are similar to those in Ref.[19] within an error of about 0.3 eV. For $Zn_{1-x}Mg_xO$ alloys, their band energy $E_{g(Zn_{1-x}M_xO)_{co}}$ (in eV) is linearly related to ZnO band energy $E_{g(ZnO)}$ and Mg content x by the following expression:

$$E_{g(Zn_{1-x}M_xO)_{co}} = E_{g(ZnO)} + xb, \tag{6}$$

where $b = E_{g(MgO)} - E_{g(ZnO)}$ is determined by the linear fitting expression and has a large difference in experimental value, for example, 1.5–1.7 in Refs.[9, 13–15, 50], 2.1-2.2 in Refs.[48, 51], and 2.4 in Ref.[52]. But our result (3.392 eV) and other calculations (2.97 eV)[23] are much larger than the experimental values as shown in Fig.5(b).

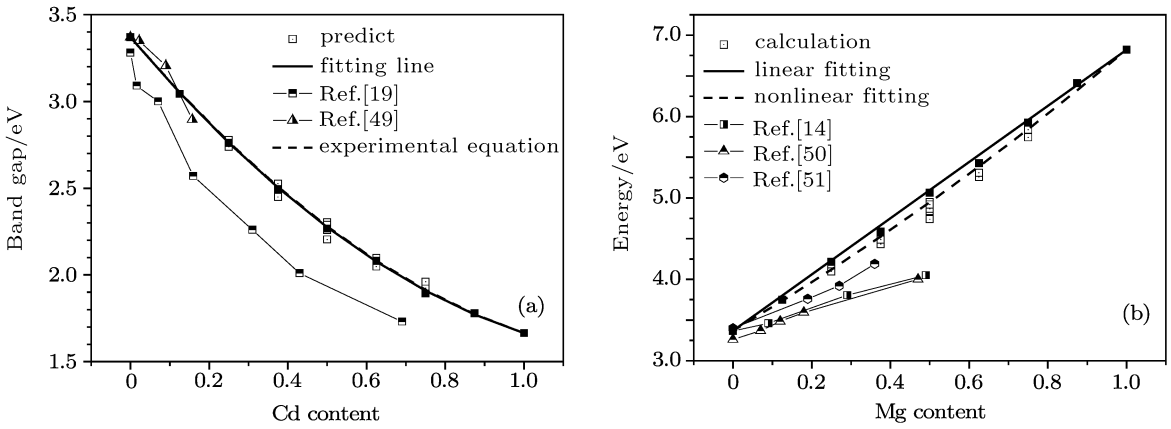


Fig.5. Corrected band gaps of (a) $Zn_{1-x}Cd_xO$ and (b) $Zn_{1-x}Mg_xO$ alloys versus Cd content and Mg content $x$respectively and their comparisons with measured and cited band gaps, as well as fitting lines.

4. Conclusion

Using DFT together with the generalized gradient corrected exchange correlation function, we have studied the structural and the electronic band properties of all possible structures of wurtzite $Zn_{1-x}Cd_xO$ and $Zn_{1-x}Mg_xO$ ($0 \leqq x \leqq 1$) ternary alloys. Our calculations show that the lengths of the a-axis and the c-axis of $Zn_{1-x}Cd_xO$ alloys linearly increase from 3.279 Å and 5.295 Å ($x = 0$) to 3.677 Å and 5.812 Å ($x = 1$) with the increase of content x respectively, which are in good agreement with other computations. For $Zn_{1-x}Mg_xO$ alloys, our calculations are in agreement with the measurements though Vegard's law does not hold true any more. The total energies, the structural and the band properties indicate the cofigurations corresponding to TD Nos. 2-1, 3-2, 4-2, 5-2, 6-1 are the possible suitable structures for both $Zn_{1-x}Cd_xO$ and $Zn_{1-x}Mg_xO$ alloys. Band gaps of $Zn_{1-x}Cd_xO$ and $Zn_{1-x}Mg_xO$ alloys are corrected and compared with the experimental values. For $Zn_{1-x}Cd_xO$ alloys, we find the corrected band gap to be in good agreement with experimental value. Our calculations and experimental values show that the band energy of $Zn_{1-x}Mg_xO$ alloys has a linear relationship with Mg content, but they have a large difference. These problems remain to be studied later.

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