

Generalized Koopmans density functional calculations reveal the deep acceptor state of N_O in ZnO

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A generalized Koopmans density functional calculation reveals the deep acceptor state of N_O in ZnO. The acceptor state is located 1.6 eV below the conduction band edge. The calculation is performed using the Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional and the generalized Koopmans density functional (gKDF) method. The results show that the acceptor state is a deep level, located 1.6 eV below the conduction band edge. This is in contrast to the shallow acceptor state of N_O in GaN, which is located only 0.3 eV below the conduction band edge. The deep acceptor state in ZnO is attributed to the presence of a localized state on the nitrogen atom, which is formed by the overlap of the nitrogen 2p orbitals and the oxygen 2s orbitals. This localized state is deep because it is formed by the overlap of orbitals with different symmetries, resulting in a strong hybridization and a deep energy level.

acceptor state in GaN.¹⁸ Here we show that the acceptor state in ZnO is a deep level, located 1.6 eV below the conduction band edge. This is in contrast to the shallow acceptor state of N_O in GaN, which is located only 0.3 eV below the conduction band edge. The deep acceptor state in ZnO is attributed to the presence of a localized state on the nitrogen atom, which is formed by the overlap of the nitrogen 2p orbitals and the oxygen 2s orbitals. This localized state is deep because it is formed by the overlap of orbitals with different symmetries, resulting in a strong hybridization and a deep energy level. We show that the acceptor state in ZnO is a deep level, located 1.6 eV below the conduction band edge. This is in contrast to the shallow acceptor state of N_O in GaN, which is located only 0.3 eV below the conduction band edge. The deep acceptor state in ZnO is attributed to the presence of a localized state on the nitrogen atom, which is formed by the overlap of the nitrogen 2p orbitals and the oxygen 2s orbitals. This localized state is deep because it is formed by the overlap of orbitals with different symmetries, resulting in a strong hybridization and a deep energy level.

Keywords: ZnO, acceptor state, deep level, gKDF, PBE, density functional theory.

²⁵⁻²⁷ The calculation is performed using the Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional and the generalized Koopmans density functional (gKDF) method. The results show that the acceptor state is a deep level, located 1.6 eV below the conduction band edge. This is in contrast to the shallow acceptor state of N_O in GaN, which is located only 0.3 eV below the conduction band edge. The deep acceptor state in ZnO is attributed to the presence of a localized state on the nitrogen atom, which is formed by the overlap of the nitrogen 2p orbitals and the oxygen 2s orbitals. This localized state is deep because it is formed by the overlap of orbitals with different symmetries, resulting in a strong hybridization and a deep energy level.

... E_N ... 2.1 eV ...

II. METHOD

... DFT ... Ref. 13 ...

$$V = \lambda$$

ee ce ab, N_0 Ref. 3 ad ec, de e e a ac-
 a f fee e. We c, c, de, e ef e, a i b i -
 a N_0 d a ead p- e c d c .
 Z. O.

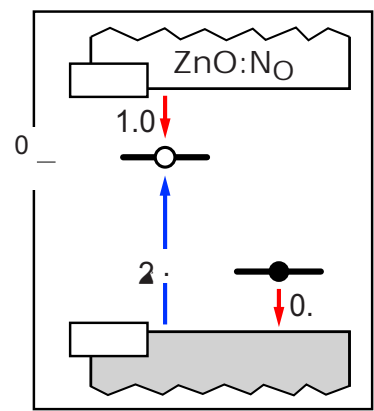
IV. HYBRID-FUNCTIONAL RESULTS FOR N_0

I de c a e e e e ca de c f e N_0
 acce . Z. O b e e de e de e e a
 V, E. 1, e de c b a ed b c d g e
 e c ca f F c e c a ge, E. 3, e f e
 e f ed b d-f. c a ca a f N_0 . S a
 e - e e a V, a b d f. c a ca, a a-
 e c ec e ca a f ge. e ae. ^{25,26}
 T ca b d-f. c a a e e ae, e e, -
 a ed b e a c e e e e ge ³⁹ a d b c. de-
 a f c a a e f c e c ²⁹ a d d . e ce a
 ec e e e a f EN, a g e e e c a-
 a e e a a e f e ed c. f acce, b d-
 g e e ge. U g e HSE b d f. c a ²⁹ a
 a ge e a a a e e $\mu=0.2$ l, e de e e e
 acce e e f N_0 . Z. O f a e f α : e
 a da d a e ³⁹ $\alpha=0.25$, f c, e e, e ba d
 ga f Z. O . de e a ed b ab, 1 eV, a d f
 a c e a ed f ac $\alpha=0.38$ c e e e e e-
 a ba d ga. ⁴⁰ Rega d. g i c a e e a d a e-
 f. c ca a e d a e NN d a ce a ge e
 . 0.02 e a e. Tabe I, e ec e f e
 c ce f e a a e e α , a d e ca a f e N_0
 acce a e e e a de ca a . Fg.
 1 b. T, e a ab, e d a e e ec c a e
 f. c a d e e i g i c a e e ba ed b
 e a f e e e a V a d b c i . f . -
 ca F c e c a ge a e ac ca de ca.
 C. de g e N_0 acce e e, e e, e be e a
 c. de a b e de e de ce e a a e e α , ba . g
 $\epsilon_A 0/ = E_V + 1.44$ a d 2.10 eV $\alpha=0.25$ a d 0.38,
 e ec e. ⁴¹ I de e a a e e e a f EN .
 e HSE f. c a, e. de e e e . -K a
 e e g $\Delta_{K} = E_{add} e_i N$ e e E. 2, ba . g $\Delta_{K} =$
 0.05 a d 0.40 eV f $\alpha=0.25$ a d 0.38, e ec e . F

ee Tabe I e a da d DFT ca a . cf. Fg. 1 .
 A a f e a a c . g a . Fg. 1 a, e e
 e N-p b a g e e a g ed a a e e
 c a c a , e e e a a a c . g a f N_0 ,
 c e de. e ed a g e f e e e
 b d . e g b . e ba a a e. We d a e
 a a c . g a . e 0.03 eV g e e e g a e
 a a ge e .
 Fg e 2 a e ca a a ed vertical a . e e-
 ge be ee. e a a $q=0$ a d . ed $q=1$ a e f
 N_0 , e.g.,

$$N_0 \Rightarrow N_0^0 + e, \quad 4$$

f e a . f e f ee-ec . e a e a
 e CBM. I a f i d e e e a . Ref. 38 a e
 EPR ac e. a N_0^0 acce ca be e c ed b g
 be e ba d ga e e ge d . 2.4 eV 514 .
 C. de g a e N acce e ed . e EPR- ac e
 ed N_0 a e bef e . a . e a g f -
 a d e e a . a e a a N acce ce a ed
 de e ca-ab . ce E. 4 f a d d ec-
 . e., e e c a . f e c a ed acce a e .
 e CBM. Q ca a a ed e e g f 2.6 eV f e ca
 a . Fg. 2 a age e e e e e e a
 e d e e g f e N- e a ed ab . ba d b e ed
 . Ref. 38. O e e e a d f e . e ce. ce . ce ,
 E. 4 bac a d d ec . e., e ec b. a . f a f ee
 e ec . e e a e f N_0^0 , e ba . a e e g f
 . 1.0 eV Fg. 2, i c a e a e e e e a
 b e ed f ee- b i d e, A^0 a . a 3.3 f eV. T, ,
 e ca . de. f . e ce. ce i b i . a N_0
 acce
 T e a ge a c e a a . ed a c a ge be e-
 ee. e a a a d . ed acce a e Tabe I e ad
 a a ge d f f e. ce be ee. e ca e ca a d e i a
 acce a . e e ge. S ec ca, e e ca
 0/1 a . Fg. 2 a d d e e acce e e
 $\epsilon_A 0/ = E_V + 1.62$ eV Tabe I. T e S e f f 1.6 eV
 c . ed f a . a e e a c . b . E_e
 0.8 eV f e e a a . e e g Ja . -T e e e g af-
 e e e ca 0 \rightarrow 1 a d 1 \rightarrow 0 a . Tabe I. We
 . e a e a a . e e ge a . d 0.8 eV a e a e ca
 f de e e a e . Z. O. S a a e a e ca a ed
 a f , e.g., L_Z Ref. 13 Z . a ca. ce. ¹⁷ T e e i a
 . a . e e g f 1.6 eV i c a ge a c .



calculated, e.g., $\Delta_{K=0} = 0.62$ eV.⁴² The band structure calculated by DFT
with the Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional
and the Heyd-Scuseria-Ernzerhof (HSE) hybrid functional is shown in
Figure 1. The band structure calculated by HSE shows a band gap of
1.44 eV, which is in good agreement with the experimental value of
1.44 eV.

a. ed V, dca, g a, - e. e. a, ca, a ge,
 acc, f e effec f, ca F c e c a, ge, ca,
 ed defec a e. T e dee, e, e f e a, - e acce,
 No a d Co a e, a, a, ca, c d, g c, -
 ce, a e, d a, a, c a ge-c, e, a e d d, -
 acce, a ca f, e, c a ged a e a d e eb
 a, e, b e dee, a e.

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T a f i, ded b e U.S. De a, e, f E. e g,
 Of ce f E. e g Ef c e, c a d Re. e ab e E. e g, r. de
 C. ac N. DE-AC36-08GO28308 NREL. T e, e f
 MPP ca ab, e a e Na, a E. e g Re ea c Sc e, c
 C, g Ce. e g a e f i, ac, edged.

¹A. T, a a, A. O, T. O, a, M. O a, T. Ma, M.
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 Y... FWA d X.

A.
 U.Hab ec, M.S. b e, a d M.D a a,
[346R](#)