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Electronic structure of the ternary chalcopyrite semiconductors
CuAls2, CuGaS2, CuInS2, CuAlse2, CuGaSe2, and CuInSe2

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The electronic structure of six Cu-based ternary chalcopyrite semiconductors is calculated self-consistently for the first time within the density-functional formalism. The chemical trends in the band structures, electronic charge densities, density of states, and chemical bonding are analyzed.

I. INTRODUCTION

There are two major groups of ternary ABX2 semicon-
ductors. Cxroup I (ternary chalcopyrites) consists of the
A 8' 'X2 compounds where 3 =Cu, Ag; B=Al, Ga,In,Tl;
and X=S,Se,Te. It is an isoelectronic analog of
the II-VI binary compound semiconductors. Group II
(ternary pnictides) consists of the f 269.56 639.89 T-6/Xi0 10.33 T52r7 12.5 4

of

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tials, '

in a conventional plane-wave basis set the problem
of obtaining a converged expansion in basis functions
would be intractable. This is so because there are no d
states in the core of the Cu atom, hence its d nonlocal
pseudopotential is purely Coulombic, '
requiring —10 —10 plane-wave basis functions. In a mixed-basis
representation, much fewer basis functions are needed (see
below). Whereas the former limit is unattainable, current
methods of matrix diagonalization (e.g., Hausholder-
Choleski methods) make even the latter limit a formidable
computational task. (iv) The lack of precise assignment of
the few lowest optical band gaps to well-defined interband transitions restricts the use of empirical fitting of the band structure, '

as done

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function variations near the nuclei) plus a set of sym-
metrized plane-wave basis functions (which describe the
weaker spatial variations in the interstitial regions). All
multicentered integrals are eliminated by using nonover-lapping compressed atom orbiials. Basis orbitals are add-
ed until the error in the band energies in the region of
Ez+10 eV is below -0.1 eV. (4) The crystal potential is described as a sum of a fixed, multicenter term (superpo-sition of renormalized quasi-atom-potentials) and a

Fourier series with adjustable coefficients p -, which G
describe all nonspherical terms. Rather than use the con-
ventional variational approach (minimize the total energy
with respect to the orbitals), we use an equivalent but computationally far more efficient potential-variation ap-
proach (minimize the

minimize

ventional

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6

-2—

{Q

Ql

C -6
LU

Cu 3d
—plus
S 3p

Q)
OP

C
Lal

-2
Cu 3d
— plus
Se 4p

-8 Ga-S Bond -8— Ga-Se Bond

- 10—

- 12—

CuGaS, -10—
- 12—

CuGaSe,
Se 4s

- 14

- 16—
Ga 3d

Fill/Ill/Ill/i F111111111111111111/i i

T N

- 16—

Ga 3d
//jjj// /jjjjj///jjj//jj/jjjj //j// /jj///// /jjj//j//jj/ //j/jj//// ////
T t N

FIG. 3. Electronic band structure of CuGaS2 and CuGaSe2 using Ceperley's correlation and the crystal-structure parameters of Table I. The principle band gap is denoted by the shaded areas.

A. The upper valence band

1. Bands

The upper valence band has its maximum at the I 4„
point in the zone center; the conduction-band minimum is
at the I ~, point, hence all six materials have a direct band gap. The4 Td (its)Tj ET BT Tf 414.44 347.1

The

materials the

upp

1. Table

valence

ELECTRONIC STRUCTURE OF... CuA1Sq, CuGaS2, CuInS2, CuAlSeq, CuGaSe~, AND CuInSe2 5827

-2

O 4

Ql

CP

LU In-S Bond

Cu 3d —plus
S 3p -4
ID

Ql
-6

La)

In- Se
Bond

O

CuGaSeU ET/Xi520 4.87 Tf 12289.67 546.33 Td5 7.08

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:::::::::::::;::::,:::::::::::::::,:::,:;:::;:::;::Conduction Band',:::::::::::::::::::;::::::::,:::::::::;:,::::::::::::::::::::::::,::::, T1c + r 2c

Y

Optical '-"-

~& & Gap

T + 3v

I ~
I
I

',

ELECTRONIC STRUCTURE OF... CuA1S2, CuGaS2, CuInS2, CuA1Se2, CuCxaSe2, AND CuInSe2 5829

TABLE III. Calculated valence-band energies at high symmetry points (in eV), given relative to the
1 4„' valence-band maximum. Notation refers to Fig. 5. The Ceperley correlation [Refs. 27(c) and 29]
and the crystal-structure parameters of Table I are used.

State CuA1S2 CuGaS2

Compound
CuInS2 CuA1Se2 CuGaSe2 CuInSe2

Upper VB
Maxima

(2) r,v
rs ~cF
T3v+ T4

~(5)

lv

0.0 —0.32 —0.67 —0.24

0.0 —0.32 —0.91 —0.48

0.0

0.075 —0.91 —0.54

0.0 —0.30 —0.76 —0.30

0.0 —0.34 —1.14 —0.58

0.0 —0.03 —1.05 —0.63
Minima

(1) r, v
T4u+ T5u

~(4)

lu

—4.63 —4.24 —4.92

—4.85 —4.37 —5.26

—5.07 —4.90 —5.41

—4.32 —4.08 —4.69

—4.74 —4.61 —5.21

—4.66 —4.64 —5.02
8"'-X '

band

r(2)

lu

I2,
(2) T5v
~(3)

lu

—4.93 —6.74 —5.99 —6.21

—5.71 —8.00 —6.82 —7.07

—5.73 —6.40 —6.29 —6.41

—4.86 —6.51 —5.81 —5.99

—6.01 —7.50 —6.80 —6.92

—5.52 —6.32 —6.15 —6.17
(1) r, v
r3u

(1) r„
Tlv+ T2v

(1) T5u
~(2)

lv
lu

—12.81 —12.83 —14.32 —12.82 —13.67 —13.05 —13.42

—12.85 —12.89 —14.87 —12.88 —14.03 —13.08 —13.77

—13.15 —13.18 —14.57 —13.18 —13.92 —13.41 —13.62

—12.49 —12.49 —13.83 —12.50 —13.23 —12.70 —13.01

. —12.81 —12.78 —14.32 —12.82 —13.65 —13.04 —13.40

—12.75 —12.75 —14.00 —12.92 —13.58 —12.96 —13.18

Center at point r

7 .

53.

70

2(91Tj ET BhaBT /Xi7 8.14 Tf 4898.56 321 (2(91/Xi.13 abouT /Xi7 8.2 BT /X9.4.67 7291)Tj2(91/Xi.13 structure)Tj ET BT /f 298.45Td (l2(91Tj ET Bsamructure)Tj ET BT /1.33 4279.)Tj2 3.444 ET 35%%uoT BT /Xi7 7.01 T T2 85 Tj ET 2(())Tj respecT BTly BT /Xi7 8.02 Tf 44287415 517Td 273.

27 .

T527 .

C7Td 273.T527 .

——

— E BT / /Xi7 12.57 Tf .447 514.11626(—)Tj ET Thn structure 1/Xi.13 ET BT /Xi7 7.69 T9.4.67 .44 ET 25(18)Tj ETstructure 818Td ([Refs2)Tj ET /Xi7 9.12 Tf 296 47.Tj /Xi2.11 18

[Refs2

structure 623u

Uppelogical/Xi7 8.08 Tf 15399.33 4(3.)Tj21 T8
UppehaBT /Xi7 8.14 Tf 48985.22 Td0d21 Td (Uppededuc ET BT /Xi7 7.71 Tf .22 35 T20CuA1S2)TjHoweveT /Xi7 7.82 Tf 1
r„

6.189.

r.89 686 ET EmplyBT /Xi7 8.55 Tf 33 Td 11 (r.89 (r)Tj j~T BT /Xi7 5.12 6T7822 3 (—)Tj179 Td ([Re=77%%uoT BT /Xi7 701 T T2.22 352d (6.179 Td ([Reconsiderabl)Tj ET BT /Xi7 9.11.67 47)Tj ET179j ET y)TjT /Xi7 8.08 Tf 15 /1.33 4212.)Tj179 Td ([RethBT BT /Xi7 7.69 T9.9.44 4 rXi.1,— r.157eV),—

r.13.

'~21 —)Tj ET Btrcture

T 4(icTcc T517 91591/Xi.13 structure 0 (—)Tj ET perceBT /Xi7 8.2 BT /X9586.67 .39j (—)Tj ET T /Xi7 12.3 Tf 4697f 867 49290.27.j ET 2 91/Xi.13 structure 5179 se7 TdT expecT 2)enoT xpc

r(2aracBT T /Xi7 12.33 Tf 37447 5142Td (l2(91TdT ET thiT /Xi7 9.9288.44 88.63 39T2 Td (5.)fir)Tsuggesd7 12.35 T 11037767 52T2 Td (5.)h(of)hpoETTj ETfor /Xi

r.329X

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Distance {a.u.}
0.0 1.0 2.0 3.0 4.0 5.0 6.9 7.9 8.0 9.9 19.911.0 0.0

9.0 1.0 2.9 3.0 4.0 5.0 6.9 7.0 8.0 9.9 19.011.012.0

1.9-

2.0-

3.0-

4.0-

5.0-

7.0-

10.0-—

9.0— I I

3 0

4.0-

OP
~ 50-
C
Cg 6.0-
CO ~~

0 70-
8.0-

9.0-

10.0-

0.0

1.0-

3.0-

5.0-

7.0-

8.0-

10.0-

FICi. 6. Calculated electronic charge density for states in the upper valence band (cf. Fig. 5). The contours are logarithm&cally spaced. (a) CuA1Se&, (b) CuA1Se2, (c) CuCxaS& (d) CuGaSe~, (e) CuInS&, and (f) CuInSe&. The solid circles denote the core regions, where the rapidly varying charge density was omitted for clarity of display.

logarithmic contours enclosing the charge of 10— e/a. u. 2 3
around the 8 and X atoms to highlight the regions that
contribute to the 8—X bond. This charge distribution
suggests that the In—X bond is considerably weaker than

the Al—X and Ga—X bonds. The B -X '

band is analo-

gous to the bottom of the upper valence band in binary II-VI semiconductors except that in the ternary analog (column-III rather than column-II cation) it is less ionical-

28 ELECTRONIC STRUCTURE OF... CuA1S&, CuGaS&, CuInS2, CuA1Se~, CuGaSe2,

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Distance (a.u.}
0.0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 S.G 9.0 10.0 11.0 0.0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.010.011.012.0

7.G-
S.G-
9.0-
10.0-
0.0
1.0-
2.0-
3.0-
5/4 6

OP

~ 5.6-
C$ 6.0-
CO

Cl 7.0-

9.0-
10.0-
0.0
1.0-
2.6-

5.0-

8.0-

10.6-

FIG. 8. Calculated electronic charge densities of the B"'-X '

2& ELECTRONIC STRUCTURE OF... CuAlS2, CuGaS2, CuInS~, CuAlSe2, CuCraSe2, AND CuInSeq 5833

Distance (a.u.)
0.0 1.0 2.0 3.0 4.0 5.0 6.

I

0 7.

I

0 8.

I

0 9.

1

0 10.

I

0 11.

I

0 0.0 1.

I

0 2.
I

0 3.0 4.0 5.0 6.0 7.0 8.Q 9.0 10.011.012.0 I I I I I I I I I I

1.0-
2.0-
3.0-
4.0-
5.0-

7.0-

9.0-
10.0-
0.0

'

1.0-
2.0-

~ 30-

40- I 5.0-

C
6.0-
~ N~

Q 70-

8.0-
9.0-
10.0-
0.0

2.0-
3.0-

5.0-

9.0-
10.0-

FIG. 9. Calculated electronic charge densities of the X '

s band (cf. Fig. 5). The contours are logarithmically spaced. The solid
circles indicate the core regions. The 10 e/a. u.'

contours around the X '

site are shaded to highlight the X '

s character of these
states. (a) CuA1Sq, (b)

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25

20-

10-

83s

Al-S

XPS
I

Main
Valence

~

I CuAIS2
Band

II

28 ELECTRONIC STRUCTURE OF... CuAlS2, CuGaSq, CuInSq, CuAlSe2, CuGaSe2, AND CuInSe~ 5835 TABLE V. Calculated (using

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10'
100=
s
CuAIS2:CBM
10-1—
C$
10-2 =
10-3
101 =
10
I
10-3
=
10-3
10-3

JAFFE10'

ELECTRONIC STRUCTURE OF... CuA1S2, CuGaS2, CuInS2, CuA1Se2, CuGaSe2, AND CuInSe2

tion of the Cu d orbitals in bonding in the upper valence band, not all of the anion p orbitals are consumed in bond-ing in the valence bands and a significant amount of anion character exists also at the CBM. The VBM ~ CBM transition in CuBXz chalcopyrites hence has an "intra-atomic" component and could be stronger than the analo-gous interatomic transition in binary semiconductors due to stronger overlap of the initial with the final-state wave functions. This also suggests that the effect of lattice thermal expansion on the temperature dependence of the

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TABLE VII. Comparison of the present band structure with that of Poplavnoi et al. {Ref.21) and Oguchi et al. (Ref. 23) at the
Brillouin-zone center. The

ELECTRONIC STRUCTURE OF... CuA182, CuCxaSq, CuInS2, CuA1Se2, CuoaSe2, AND CuInSe2

TABLE VIII. Calculated x-ray scattering factors of the six group-I ternary chalcopyrites, in units of e/cell. The reciprocal-lattice vectors are divided into three groups [(i)-(iiii]. Group (i) denotes the zinc-blende-like factors, group (ii) denotes the anion factors (van-ishes for Q = 4), and group (iii) denotes the cation ionicity factors, cf. Eqs. (1)—(3). The maximum error bars are estimated at
+0.3e/cell.

Reciprocal-lattice
vectors

Group (i)
0,0,0
1,1,1
2,0,0
0,0,2
2,0,2
2,2,0
1,1,3
3,1,1
2 2 2

4,0,0
0,0,4
3,3, 1
1,3,3
2,0,4
2,4,0
4,0,

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220—
210—
200-
190 =-
180—
170—
160—

140—
130—
120—
110-
100—

50—
40-

20—

50

40

30

20

10

0.6—

0)
V

30
V
5$
LL 10

V

0)

60
C$
'PC

I

Zinc-blende-like
StrUctUre Feet&r&

[2,2,0]

[4,0,0]—

[3,3,1]

[2,4,0]

[2,2,2]
[2,0,0]

I I

1,0,3/2]
1,0,5/2]

and p&(G)=ps(G) =,

[f—z(G)—fz(G)]g3". We hence
refer to p2(G) as the "anion factor" and to p3(G) as the
"cation ionicity factor. "
Table VIII lists the calculated x-ray scattering factors of the six group-I ternary chalcopyrites, arranged ac-cording to the three groups of reciprocal-lattice vectors. In the calculation we have not assumed that the charge density in the crystal can be approx.22 633 Torranged

be

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p(r) can be described as a superposition of spherical
atomic charge densities p'" (r —r) at sites r. In con-
trast, the full band-structure calculations make no use of
such simple approximations and hence produce a nonzero

bonding charge

A(r)=p(r)—gp~" (r —r).

Distance (a.u.)

0.0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 0.0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.010.011.012.0 0.0

I I I I I I I I I I I I I I I I I I

1.0-
2.0-
3.0-
4.0-

6.0-
7.0-

10.0-
0.0
1.0-
2.0-
3.0-
4.0-
OP 5.0-
6.0-
th ~ ~
Cl 7.0-
8.0-
9.0-
10.0-

3.0-
4.0-

6.0-

8.0-
9.0-
10.0-

FIG. 15. Contour plots of the total valence electronic charge density of the six group-I tenary chalcopyrites. The contours are log-
arithmically spaced. The solid circles denote the core regions. The 8)&10 to 10 '

e/a. u. contours are shaded to highlight the co-
valent A'—X '

bond. (a) CuAlS2, (b) CuA1Se2, (c) CuGaS2, (d) CuGaSe2, (e) CuInS~, and (f) CuInSe2.

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e can devise an approximate procedure to

EI,ECTRONIC STRUCTURE OF... CuAls2, Cueas2, CuIns2, CuA1se2, Se CuGaSe, AND CuInSe2 5843

hkl

M

hkl iogtoTz = g logioT M

(7)

For the ternary chalcopyrites examined we find that T2 is
within 5% of the more exact

4indEC67(4ind)TRBT 551i18.52 Ta541567 614.337)C67(4ind)TT 593i21 9.26TTf 253.14.56 184GaS767(4ind)TwhicT 0321 9.07 .68 164T4 6254(M)Tj

4ind

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functions in the solid, highlighting the transferability of

these radii. d, „denotes in Figs. 16 and 17 the distance
from the anion sites (in units of the corresponding bond
distances) at which the charge density reaches its max-
imum pm»
A number of chemical trends are evident. First, the charge along the 3—X bond is generally more polarized towards the anion site than the charge along the B—X bond, i.e., dm» &dm», suggesting the higher polarity of the 3-X charge distribution relative to the B-X distribu-tion. Second, whereas the sequence of increasing polarity
(i.e., decreasing d,„) along the A

'—X '

bonds is

In&Cd&A1, the sequence is reversed along the B"'—X ' bonds, i.e., Al&Ga&In. The peak values of the bond charge densities pm» follow the trends p~',„&p~',„ &pm~a. Hence, among the sulfides, CuA. ISz has the most ionic A—X bond and the least ionic B—X bond, whereas CuInS2 has the least ionic A—X bond but the most ionic B—X bond. It is therefore not meaningful to ask which of the CuBX2 sulfides or selenides is the most ionic?" since the answer is dif.trent for each of the two bonds in the system. These trends agree remarkably well with the

model bond ionicities calculated by Levine '

from the

dielectric theory of ionicity, as well as with the observed trends in the nonlinear optical susceptibilities. Third, the sulfides have a larger bond polarity than the selenides

both in the A-X and in the 8-X contacts (i.e., d,„&d and d,„&d,„'). Fourth, whereas the 8 Xbond ch—arge
is localized between two minima near the X and B sites, respectively, the A —X bond charge is confined by a densi-ty minimum only near the anion site. The shaded areas in Figs. 16 and 17 highlight these different asymmetries be-

tween the two basic chemical bonds and suggest the higher stability of the Cu-X contact relative to the 8-X
contact.

IX. ADJUSTING THE BAND STRUCTURE

As seen from Table V and discussed in the Introduc-

tion, the local-density formulation of interelectronic in-
teractions underestimates the optical band gaps relative to experiment. %'hile many of the chemical trends in the
electronic structure can be studied by using the local-
density approach, investigation of the variations in the
band gaps (e.g., with structural parameters) clearly re-
quires that it will have a physically correct magnitude. This can be done in an ad hoc fashion by scaling the ex-
change coefficient a. We find empirically that
a=1.0—1.1 produces the correct optical gaps in these compounds. For example, Fig. 18 compares for CuInSez the band structure obtained by using Ceperley's correla-
tion with the band structure obtained by using an ex-
change coefficient a=1.1. Table X compares the band
energies in these two calculations. It is seen that upon
scaling the exchange coefficient the Cu d components of the upper valence band move to more negative energies
relative to the original calculation, leading to an opening
up of the optical band gaps due to the reduced I »(d)- I »(p) repulsion (cf. Sec. IIIA). Scaling up the exchange coefficient increases the attractiveness of the crystal po-
tential in regions of space of high charge density and
therefore lowers the localized states (e.g.,

the 8"' d band
and the X '

s band) more than the extended states {e.g.,
the upper valence band). This exercise clearly indicates

TABLE X. Comparison of the band structure of CuInSe2 calculated with the Slater exchange (using
+=1.1) and with the Ceperley exchange correlation "' (XC). Results (in eV) given relative to the I 4,'
valence-band maximum. Results for Slater exchange with a= 1.0 were given in Ref. 25.

State

Upper VB
Maxima
(2)
I

(2)
Sv

3u+ 4u

~(S)

Slater
exchange

0.0 —0.08 —0.79 —0.54

Ceperley
XC

0.0 —0.03 —1.05 —0.63

State

X 's band

(1) I Su

I 3v r("1u
T1u+ T2v
(1)

TSU

Slater
exchange

—13.03 —13.06 —13.83 —13.00 —13.46

Ceperley
XC

—12.75 —12.75 —14.00 —12.92 —13.58

Minima

(1) I 4v
T4v+ TSu

~(4)

1u

—5.15 —5.12 —5.13

—4.66 —4.61 —5.02

~(2)

1v ~(1)
1v B"' d band

—13.20 —13.31 —21.48

—12.96 —13.18 —16.93
8"'-X

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that there does not exist a single exchange coefficient o. that produces a correct optical gap and the correct energy positions of the localized bands. However, this empirical device of scaling up the exchange coefficient is adequate for the restricted scope of studying the variation of the band gap with structural parameters. Taking CuInSe2 as an example, we find that although the band gap increases with exchange scaling (Es———0.2 eV using Ceperley's
correlation and Eg:0.98 eV using Slater's exchange
a =- 1.I), its structural derivative dEs/du is similar in both cases (18.2 and 21.1 eV for Ceperley's and Slater's func-tionals, respectively). This suggests that one can use a scaled exchange for the restricted objective of producing nonvanishing band gaps for the

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