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TABLE I. LDA calculated conduction-band energies (in eV, relative to valence-band maximum) at some high-symmetry points of zinc-blende and wurtzite semiconductors. Results are calculated at the experimental lattice constants (Ref. 4) ao (in A) using the LAPW (L) method or the pseudopotential (P) method with core correction. In both cases, we use the LDA exchange-correlation potential of Ref. 10. An asterisk denotes the lowest band gap.

Type Compounds

Zinc-blende

eigenvalues (eV)

Lq,

Wurtzite

eigenvalues (eV)

M1 Ui,
I
II
II
II
II
II
II
II
II
II
II
II
III
IV
IV
IV
V

GaSb(P)
GaN(L)
GaAs(P)
InN(L)
ZnO(L)
ZnS(L)
ZnSe(L)
ZnTe(L)
Cdo(L)
Cds(L)
CdSe(L)
CdTe(L)
AlN(L)
AlAs(P)
AIP(P)
SiC'(L)
Gap(P)

6.0959
4.5094
5.6532
4.9882
4.5707
5.4102
5.6676
6.0990
5.4217
5.8180
6.0840
6.4810
4.3714
5.6600
5.4670
4.3590
5.4506

0.12*
1.76*
0 44+
—0.38*
0.63*
1.86*
1.05*
1.04*
—0.41*
0.87*
0.31*
0.50*
4.24
1.90
3.10
6.30
1.76

0.82
3.29
1.36
2.87
5.18
3.22
2.84
2.17
4.62
3.32
2.96
2.49
3.25*
1.35*
1.50*
1.32*
1.56*

0.39
4.56
0.94
3.04
5.35
3.09
2.36
1.64
3.51
2.76
2.16
1.63
7.28
2.02
2.69
5.39
1.63

0.13
1.91*
0.47*
—0.26*
0.71*
1.95*
1.10*
1.04*
—0.36*
0.94*
0.38*
0.54*
4.36*
1.93
3.14
6.31
1.81

0.02*
4.18
0.57
2.78
5.14
2.86
2.12
1.35
3.39
2.58
1.99
1.43
6.88
1.64
2.27
4.67
1.23*

0.67
4.94
1.20
3.76
5.67
3.47
2.93
1.98
3.63
3.51
3.02
2.30
5.66
1.62*
1.83*
2.64
1.42

0.54
4.01
1.05
3.04
5.31
3.16
2.56
1.82
3.81
3.01
2.51
1.94
4.90
1.66
2.03
2.98
1.51

'SiC in the wurtzite structure has a minimum LDA energy gap of 2.15 eV at K.

eV)

Ref.

5. 6t

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transition is predicted for Gap where L,', state is close to the
conduction-band minimum at X&, (see Table I).
In summary, we have found three simple rules to predict
the basic band-structure type of a wurtzite octet compound
from its zinc-blende energy levels. We explained the small
direct band-gap differences between the zinc-blende and
wurtzite structure in a type-II system and large indirect gap
differences in a type-IV system. We also predict that as the lattice changes from zinc blende to wurtzite an indirect-to-

direct transition will occur in A1N, an indirect-to-
pseudodirect transition will occur in GaP, and a direct-to-
pseudodirect transition will occur in GaSb. Experimental
investigations on these predictions are called for.

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