VOLUME 41& NUMBER

1 PHYSICAL RKVIKW LKTTKRS

VOLUME 4I, NUMBER 1 PHYSICAL REVIEW LETTERS 5 JULY 1978

tential Vs"'(r) = V, (r) —Z„/~+& (& + 1)/~' as

VFP~'~(r) =(U, (y)+l(l ~1)/2x'] —Z„/x +V„,[p']+(V„[p'+p"] —V„,[p'] —V„,[p "J}+(V„[p"]-V„[n"D +(V„,[p "J - V„[n"J),
where the repulsive potential U, (x) is given by

(2)

)~„'C~.n' (en& —en't)4n't (&)
U~(r =

The first term in the curly brackets contains the nonlocality while the rest of the terms

VOLUME 41, NUMBER 1 PHYSICAL RKVIKW LKTTKRS 3 JUz, v 1978

3.5

3.0—

2.5—

vKF

I

RbF

aO

RbCI v

v KCI
RbBr
aS
v KBr

Cesium chloride

t CsCI

t CsBr

30

2.5—

2.0—

v BaSe
SrSe

Rbl v

t Csl

2.0—

g 1.5
b
M

1.0—

InN g
Z 0 AgC
WurtzitB Hgs I

'~C
AgBr &
AIN ~ ~I

Na

HgSe CdSe
CuCI QMgS
SiC ZnS&& l

L

g—inp gg(MgS~

BeTe Gap 0

0
AIPO
GaAs0

BN o Z b

AIAs &&
BeSe AISb

GaSb o-()BeS—e-~~.
Si Ge Sn
Diamond

Zinc blende
~ Diamond

Graphite ' Wurtzite
& Rocksalt
Cesium chloride

1.5—

0
b

1.0—

0.5—

0—

—0,5—0.5

AuC

Ca

BaCd
SrCd
BaHg

I I

0.5 1.0

R~ (a.u.)

o BeCu
Cd
LiG aBi
CaH NaPb

MgAu ~Ca
Liln

Na Tl ~ Ltpi

n ~ LiZ n
g g

BITIO LiTI~~, I I

o P LiCd CuZn CdAg~
Mg Tl LiHg~ LiAg

Au

o CsAu

I

1.5

~ L10
o B32
o B2
& B33
~ tl64
~ CP64

2.0

—0.5
—0.5

I

0.5

R~ (a.u.)

1.0

I

1.5 2.0

FIG. 2. R~ vs R~ plot for the suboctet binary con-pounds. The separation lines are included for conven-ience.

FIG. 1. R~ vs R~ plot for the octet binary coznpounds. The separation lines are included for convenience.

provide a better structural sensitivity.

"

The separation of the suboctet compounds works well not only for the two broad classes of bcc-
like structures (full symbols) and the anion-val-
ence coordination compounds (open symbols) but
also for a large part of the various space groups appearing in these systems. Of the exceptions we note that AuCl (L10), CaAg (B33), and NaPb (tI64) have unusual properties.

"

In order to study the quality of our first-princi-ples potentials away from the turning-point re-gions, we apply it to electronic structure prob-
lems which are sensitive to lower-momentum

components. A nonlocal (l =0, 1, 2) self-consis-
tent band study on Si, using the Kohn-Sham ex-change and the free-electron correlation poten-tial, yields results that agree very well with all-electron first-principles calculations and with
photoemission studies. We obtain a bandwidth of
12.40 eV (observed 12.4+ 0.6 eV) while the loca-

tions of the high-symmetry valence states are

L,„(1.39 eV), X,„(3.13 eV), L „„(7.09 eV), L,.„ (9.85 eV), and &, ~„(4.80 eV), compared with the observed values'4 of 1.2+ 0.2, 2.9+ 0.3, 6.4 +0.4, 9.3+0.4, and 4.7+0.3 eV. The "forbidden" [222] x-ray scattering factor is 0.112ejatom, compared with the observed value of 0.119. The ground-state charge density has the expected anisotropy,

"

i.e., elongated parallel to the band
axis, with an anisotropy ratio of 1.62, compared with the observed value" of - 1.4-1.5 and the self-

consistent empirical pseudopotential value of 0.8
(local) and 1.2 (nonlocal, non-self-consistent").
We have performed similar studies on Ge" and
Mo" and obtained comparable results. We con-
clude from the present study that the density-
appref 473.28 173.23 Td . funetional pseudopotential approach correctly

Vox.UMz 41, NUMsxR 1 PH YSICAL REVIEW I.KTTKRS $ JULY 1978

tures can be cast in the simple analytic form
—Z„/r+&&(& -yp) + &(&+ &)/2r' used by Andreoni
et 4.' as can be evidenced from the similarity of
the radii for the first-row atoms.

"

This would

enable a convenient use of these potentials for a wide range of electronic and structural proper-ties.

We thank Dr. J. C. Phillips for sending us pre-prints of beefs. 6 and 13. This work was supported in part by the Division of Basic Energy Sciences, U. S. Department of Energy, and by the National
Science Foundation under No. Grant No. DMR76-20647-A01.

'M. L. Cohen and V. Heine, in SoEM State Physics, edited by H. Ehrenreich, F. Seitz, and D. Turnbull (Academic, New York, 1970), Vol. 24, p. Q8.
~G. Simons, J. Chem. Phys. 55, 756 (1971).
G. Simons and A. N. Bloch, Phys. Bev. B 7, 2754 (197').
4J. St. John and A. N. Bloch, Phys. Rev. Lett. 83, 1095 {1974).
E. S. Machlin, T. P. Chow, and J. C. Phillips, Phys, Bev. Lett. 38, 1292 (1977).
J.R. Chelikowsky and J. C. Phillips, Phys. Rev. Lett. 89, 1687 (1977).
'A. B.Miedema, F. R. de Boer, and P. F. de Chatel,

J. Phys. F 8, 1558 (1978).
W. Andreoni, A. Baldereschi, F. Meloni, and J. C. Phillips, Solid State Commun. 25, 245 (1978).
~G. Simons, Chem. Phys. Lett. 18, 815 (1978).
A. Zunger, S. Topiol, and M. Ratner, to be pub-lished; A. Zunger and M. Batner, to be published.

'L. R. Kahn, P. Baybutt, and D, G. Truhlar, J. Chem. Phys. 65, 3826 (1976).
A. Zunger and M. L. Cohen, to be published.
~J. R. Chelikowsky and J. C. Phillips, Phys. Rev. B 17, 2453 (1978).
~4W. D. Grobman and D. E. Eastman, Phys. Rev. Lett. 29, 1508 (1972); %. E, Spicer and R. C. Eden, in Pro-ceedings