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Publication Date

1974-11-01

Submitted to Physical Review

LBL-3540
Preprint C. 1

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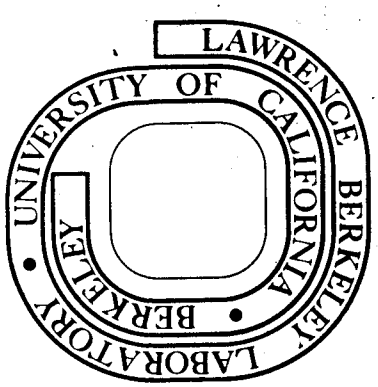
November, 1974

Prepared for the U. S. Atomic Energy Commission
under Contract W-7405-ENG-48



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An Alternative Form of the Nonlocal p-Potential in the Empirical Pseudopotential Method

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Abstract

An alternative nonlocal p-potential is suggested. The energy gaps at a few important k-points are calculated for NbC and NbN and compared with previous results.

Recently, we have calculated the band structures of NbN[1] and NbC.[2] Since the anions in these two compounds are in the first row of the periodic table, they do not have core p-states. From the point of view of the Phillip's

cancellation theorem, the valence p-states of C and N are not cancelled by the core states of same character. Because of this, in our previous calculations,[1,2] we have augmented the potential with an $\ell = 1$ nonlocal pseudopotential having the following form:

$$V_{NL}(\underset{\sim}{r}) = \sum_j \hat{P}_1^{+} U(|\underset{\sim}{r}-\underset{\sim}{R}_j|)\hat{P}_1 \qquad (1)$$

where $\hat{P}_1$ is a projection operator which operates on the spherical harmonics with $\ell = 1$, and $\hat{P}_1^{+}$ is the corresponding Hermitian adjoint operator. The form of $U(|\underset{\sim}{r}|)$ is

$$U(|\underset{\sim}{r}|) = \begin{cases} A_1 r e^{-\alpha r} & r \leq R_s \\ 0 & r > R_s \end{cases} \qquad (2)$$

where R_s is the core radius of the atom. A_1 and α are treated as disposable parameters. When Eq. (1) is evaluated between two plane waves, we get the following radial integral in the matrix elements:

$$\int_0^{R_s} j_1(k_1 r) j_1(k_2 r) r^3 e^{-\alpha r} dr \qquad (3)$$

where k_1 and k_2 are the magnitudes of $\underset{\sim}{k}$ for the two plane waves. Because the integrand is singular as $r \to 0$, the integral does not have a closed form. A gaussian quadrature numerical integration routine with 8-point has been used in refs. 1 and 2. Unfortunately, we have found that the 8-point integration scheme is not highly accurate and the effect of the p potential is over estimated. To avoid the singular

behavior in the matrix elements, we suggest here an alternate form for the nonlocal p-potential:

$$V_{NL}(\underset{\sim}{r}) = \begin{cases} \sum_j |U_1(|\underset{\sim}{r}-\underset{\sim}{R}_j|)P_1\rangle\langle U_1(|\underset{\sim}{r}-\underset{\sim}{R}_j|)P_1| & |\underset{\sim}{r}-\underset{\sim}{R}_j| \leq r_s \\ 0 & |\underset{\sim}{r}-\underset{\sim}{R}_j| > r_s \end{cases} \quad (4)$$

where $U_1(r)$ is a constant. The differences between the present form and Eq. (1) are: (a) The radial part of the potential in Eq. (4) is nonlocal; (b) The matrix element of Eq. (4) between any two plane waves can be expressed in closed form, and therefore, there is no need for a costly numerical integration routine.

The value of $U_1(r)$ is determined by fitting the important p to s and d energy gaps reported in ref. 1 and 2 by keeping R_s, the local and the d nonlocal pseudopotential fixed. In table I, we compare the values of the previously obtained energy gaps with the ones calculated by using Eq. (4). In NbC, the overall difference is of the order of 0.2 eV. The largest discrepancies in NbN are at X_5, and L_3. The better overall agreement for the NbC case is probably due to the fact the A_1 used in ref. 2 was about 0.5 ryd. smaller than that used in ref. 1.

Part of this work was done under the auspices of the U.S. Atomic Energy Commission.

References

* Supported in part by the U.S. Air Force Office of Scientific Research (AFSC) under Grant No. AFOSR-72-2353.

† Supported in part by the National Science Foundation Grant DMR72-03206-A02.

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2. D. J. Chadi and M. L. Cohen, Phys. Rev. B10, 496 (1974).

Table Caption

Table 1. Comparison of the principal energy gaps in NbC and NbN for two forms of the nonlocal p-pseudopotential.

Table 1

Compounds	NbC		NbN	
nonlocal p-pseudopotential	Eqs. (1) and (2)	Eq. (4)	Eqs. (1) and (2)	Eq. (4)
$\Gamma_{15} \rightarrow \Gamma_1$	4.06 eV	3.75 eV	6.52 eV	6.52 eV
$X_{4'} \rightarrow \Gamma_{15}$	3.08	3.15	2.25	2.21
$X_{5'} \rightarrow \Gamma_{15}$	0.98	0.99	0.9	0.41
$\Gamma_{15} \rightarrow \Gamma_{25'}$	0.92	0.79	1.14	1.14
$\Gamma_{15} \rightarrow \Gamma_{12}$	3.08	2.96	3.14	3.14
$L_1 \rightarrow \Gamma_{15}$	5.23	5.45	4.84	4.6
$L_3 \rightarrow \Gamma_{15}$	4.96	5.39	4.21	5.23
$X_3 \rightarrow \Gamma_{15}$	2.15	2.35	1.74	1.74
$\Gamma_{15} \rightarrow X_1$	2.58	2.4	2.68	2.69
$R_1(r)^2$		-0.19 ryd		-0.67 ryd

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