Local-Density-Functional Approach to the Self-Consistent Properties of Solids: Diamond, BN, and LiF

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1. Introduction

[redacted]

…local-space parts have indicated the large degree of variational flexibility offered by a nonlinearly optimized (exact) numerical atomic-like basis set. We

…properties…

role of exchange and correlation [11, 12]. Compa…

…particle eigenvalue equation for a periodic…

We outline here only those aspects pe… is to solve the local-density one-…

…basis functions … taken as exact numerical solutions of the single-site LDF one-particle equation … first-row atoms … 1s, 2s, 2p, 3s and 3p orbitals for the band calculation …

The matrix elements of … in the Bloch basis … by direct three-dimensional Diophantine numerical integration [10] without

... a reasonable ... charge in the background space.

... depends critically on the basis set ...

orbitals ... responsible for a nonnegligible amount of charge in the interionic region ... at the bond center compared with ... values of 0.15–0.20 ... while a simple description of the solid in terms

estimate of the equilibrium lattice ... found to be essential for an accurate ... constant.

... the static ... obtained here by a ... the variational crystal density onto a set of ionic ... densities with fractional charges ... A different picture emerges ... of the dynamic ...

... neighbors only. This neglects the ... summed over ...

... ion–ion orthogonality terms, the approximation ... ionic charges are not radially distorted in the interacting system, and that the

[redacted]

forces are neglected.

[redacted]

(the omitted repulsive potential being slightly larger) and tend to cancel each other.

[redacted]

Further analysis of the model was carried out to understand the nature of the requisite terms. We have calculated the total energy of LiF in crystal using a non-self-consistent superposition density made up from free-ion local density orbitals. The potential energy terms *PE* (Coulomb exchange and correlation) were directly calculated from this density while the kinetic energy term

between the [redacted] terms in and the attractive potential terms

kinetic terms in ... Finally, when approximation iii is removed in a fully self-consistent calculation

with experiment in a simple ... [redacted] lax the underlying

approximation ... calculated crystal density).

...

...mation from gaseous N_2 and ... crystalline boron was determined [A. ... ; see also G. ... and W. E. Wilson, Nature 191, 380 (1961)] to be 60.7 ± 0.7 kcal/mol at 298 K. Correcting the ionization energy of nitrogen and boron [L. Pauling, *The Nature of the* ...

19. H. D. Hagstrum, Phys. Rev. 72, 947 (1947); *JANAF Tables* ... D. Stull, Ed. (Dow Chem..., Midland, Mich., 1965) ... data. The heat of fo... Berl a...

[illegible] for cooling to 0 °K [illegible] data from D. R. Stull, Ed., *JANAF Tables of Thermochemical Data* (Dow Chemical Co., Midland, Mich., 1965)] and finally for the zero-point energy of the solid [using a Debye equation with θ_D = 1700 °K using data given by P. J. Gielisse, S. S. Mitra, [illegible] R. Marshall and E. A. Pascoe, Phys. Rev. 155, 1039 (1967)], one obtains an estimate of [illegible] eV [illegible] for the static cohesive energy. The accuracy of this quantity is at present difficult to assess.

[illegible] H. W. Ch[illegible], J. Chem. Phys. 26, 916 (1957).

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