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Calculation of Electronic and Optical Properties of Diamond for Wurtzite Crystal

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Abstract: *The main objective of this paper is to have a comprehensive set of results obtained by a state of the art method that could be the basis for their studies in Wurtzite materials. Frequency dependence of the dielectric function is computed within the random phase approximation. We have applied the 3d orbitals such as Wurtzite Zinc oxide, we can complete the Gw calculation with 32k points in Brillouin Zone within 3 days. The Gw band gap of Zinc oxide is smaller than experimentally obtained value. In this present paper we calculate electronic and optical transition of diamond for wurtzite crystal.*

Keywords: *Eigen Functions, Brillouin Zone, Gw Calculation, Green Function.*

I. INTRODUCTION

The semi-ab-initio approach with a minimal basis set gave results far more superior than the semi empirical tight binding method with only a modest increase in computational effort. The transferability of the basis set and the potential makes it ideal for studying more complex configuration of the semi conductor systems and compounds or for more demanding calculations such as non linear optical properties.

Almost all of the tin wurtzite crystals are materials of increasing importance in modern technology. BeO is a pyroelectric material composed of very high elements BN and SiC are known for their superior mechanical properties that are especially valuable in high temperature applications.

Although the stable phase of BN is the hexagonal phase and SiC has a number of polytypes with ZB being the most common one, the wurtzite phase is important in connection with stability in the epitaxial growth of thin films and in the structural phase transitions under pressure.

The Kohn-Sham forms of the exchange correlation potential with Wigner interpolation formula for additional exchange effects were used. I have applied a full basis set consisting of linear combinations of atomic orbitals expressed as sum of Gaussian type orbitals. In the calculation the 3d orbitals of Al, Ga and Se and the 4d orbitals of Cd and In were treated as valence orbitals.

Extra orbitals corresponding to excited states for each atom were included to ensure sufficient convergence in the basis set expansion. For the optical calculation, the real part of the frequency dependent inter band optical conductivity was evaluated first with all the optical transition matrix elements between the unoccupied valence bands and the occupied conduction bands.

II. RESEARCH MODEL

A. Local Density Approximation Potential And Linear Combination Of Atomic And Orbital

The calculations discussed below are nonrelativistic. They are performed at zero temperature. The only effect of temperature that is considered is that obtained by using the applicable lattice parameters. Our calculations utilized an expanded version of the electronic structure calculation program package from the Ames Laboratory of DOE in Iowa. Details of the computational method are available in several previous publications.

We employed the Ceperley-Alder type of local-density potentials as parametrized by Vosko, Wilk, and Nusair. The above referenced publications describe the general features of our method, i.e., the LDA potential and the standard implementation of the LCAO.

We discuss below our distinctive implementation of the LCGO or LCAO method in a fashion that circumvents the basis set and variational effect noted above.

B. Bagayoko, Zhao and Welliam's Procedure

In a typical *ab initio*, self-consistent calculation that employs the LCAO method, electronic eigenfunctions are expanded using basis sets derived from atomic calculations. Charge densities and potentials are constructed. The Hamiltonian matrix is generated and diagonalized. Key output quantities are energy levels or bands and related wave functions. The resulting output wave functions - for the occupied states - are employed to generate a new charge density and the computations are repeated. The process of using the output of iteration (n) - for occupied states - to construct the input for iteration ($n + 1$) continues until self-consistency is reached. Various measures are utilized to define self-consistency, i.e., when basic quantities, including charge densities, potentials, eigenenergies, etc. are, respectively, unchanged from one iteration to the next.

The trial basis sets are found by various authors by augmenting the atomic orbitals with polarization and diffuse orbitals whose numbers, until the work of Bagayoko, Zhao, and Williams¹ and Bagayoko et al., had no particular limit. In fact, from a completeness standpoint, the larger these numbers the better, provided no "catastrophic sinking of energy levels" or negative Millican population numbers occur for occupied states. The BZW procedure suggests a minimum of three self-consistent calculations that utilize basis sets of different size. It generally begins with the minimum basis set, i.e., the basis set needed to account for all the electrons of the atomic or ionic species that are present in a molecule, a cluster, or a solid. In the case of GaN, we chose these species to be Ga^{1+} and N^{1-} . Completely self-consistent calculations are carried out. For the second calculation, the minimal basis set is augmented with one or more atomic orbitals that belong to the next and lowest-lying energy levels in the atomic or ionic species. The self-consistent bands from calculations I and II are compared, graphically and numerically. In general, there will be qualitative (shape and branching) and quantitative (numerical values) differences between the occupied bands from calculation I and II. A third calculation is performed, using the basis set for calculation II as augmented with orbitals representing the next lowest-lying atomic energy levels. This process is continued until the comparison of the occupied energy levels leads to no qualitative or quantitative difference. When the result from calculation N and those from calculation (N+1) agree within the computational error then the optimum basis set is that of calculation N. This selection rests on the fact that a lowering of unoccupied levels, as in calculation (N+1), after the occupied levels converged with respect to the size of the basis set, as in calculation N, could be a mathematical artifact. Such a lowering may not be the manifestation of any fundamental interaction, but rather the expression of the basis set and variational effect identified above. This assertion is partly verified by computational experiments reported in Sec. III A. In multispecies systems like GaN, two or more orbitals may be added at a time if the affected atomic levels are close in energy. While we utilized the occupied energy bands for the determination of convergence with respect to the size of the basis set, we suspect that other parameters could be employed. They may include the charge density for occupied states and particularly the potential.

III. COMPUTATIONAL DETAILS

The wurtzite GaN belongs to the C_{6v} group. We considered two sets of lattice parameters for GaN. The low-temperature values we selected are $a = 3.16$ Å, $c = 5.125$ Å, and $u = 0.377$, where u is the distance between the Ga plane and its nearest-neighbor N plane in the unit of c . Even though our calculations are for zero temperature, we also performed calculations for experimentally measured lattice contents for room temperature, where $a = 3.1878$ Å, $c = 5.1850$ Å, and $u = 0.375$. In the C_{6v} group, the Ga and N atoms are in $(2b)$ positions as follows: Ga, $(0, 0, 0)$, $(1/3, 2/3, 1/2)$; N, $(0, 0, u)$, $(1/3, 2/3, 1/2, + u)$. The atomic wave functions of the ionic states of Ga^{1+} and N^{1-} were constructed from the self-consistent, *ab initio* atomic calculations. The radial parts of the atomic wave functions were expanded in terms of Gaussian functions. A set of even tempered Gaussian exponents was employed with a minimum of 0.166 and a maximum of 0.5585×10^5 in atomic unit. We used 19 Gaussian functions for the s and p states and 16 for the d states. A mesh of 24 k points, with proper weights in the irreducible Brillouin zone, was used in the self-consistent iteration calculations. The computational error for the valence charge was about 0.00022 for 52 electrons. The self-consistent potentials converged to a difference around 10^{-5} after about 35 iterations. The total number of iterations varies with the input potentials. In the self-consistent LCAO calculations for Si in the diamond structure, we used the experimental lattice constant of $\alpha = 5.43$ Å in the calculations. The atomic wave functions were constructed from results of self-consistent, *ab initio* atomic calculations. The radial parts of the atomic wave functions were expanded in terms of Gaussian functions. A set of even-tempered Gaussian exponents was employed with a minimum exponent of 0.099 and a maximum of 0.65×10^6 in atomic units. We included 19 Gaussian orbitals in the basis set for the expansion of the

atomic wave functions of Si. For the extra atomic wave function of Si ($3d^0$), we used 15 Gaussian orbitals. In the self-consistent calculations, we included 60 general k points in the irreducible Brillouin zone with proper weights. The computational error for the valence charge was about 0.000 95 for 24 electrons. The self-consistent potential converged to about 10^{-5} . Diamond (C) has a lattice constant of $a = 3.567$ Å. The bond length of the C-C nearest neighbour is 1.545 Å, which is much shorter than the Si-Si bond length of 2.351 Å. The Gaussian functions we used to expand the carbon atomic wave functions have a minimum exponent of 0.12 and a maximum of 0.1×10^6 . Sixty k points were used in the self-consistent electronic structure calculations. Ruthenium dioxide (RuO_2) is a member of the transition metal oxide family. RuO_2 has a rutile structure and exhibits metallic conductivity. Tetragonal RuO_2 has the symmetry of the $p4_2/mmm (D_{2h})$ space group. RuO_2 has six atoms per unit cell, two ruthenium and four oxygen. The ruthenium atoms are located at the Wyckoff 2 (a) sites: $(0,0,0)$ and $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$. The oxygen atoms occupy the Wyckoff 4 (f) sites: $\pm(u + \frac{1}{2}, \frac{1}{2} - u, \frac{1}{2})$ and $\pm(u, u, 0)$. The lattice constants of ruthenium dioxide are $a = 4.492$ Å $c = 3.106$ Å and $u = 0.306$. The basis sets for each of the five self-consistent calculations used in the BZW procedure are indicated in Table 1. The optimal basis set for the RuO_2 calculation is basis set II in Table I. A total of 25-37 iterations were necessary for convergence. The convergence of the potentials was up to 10^{-5} . We considered 60k points in the irreducible wedge of the Brillouin zone.

IV. ELECTRONIC PROPERTIES AND OPTICAL TRANSITIONS OF DIAMOND

The BZW procedure leads to an optimum basis set of $\text{C}(1s2s3s2p)$ for the LCAO calculation for diamond. Here, the $\text{C}(3s)$ orbital is empty. The calculated electronic band structure of diamond is shown in Fig. 1. The top of the valence band (band edge) is at the Γ point. The bottom of the conduction band is near $(2\pi/a)(0.81, 0, 0)$. The calculated indirect band gap (E_g) is about 5.05 eV, which is close to the experimental value of about 5.3-5.48 eV. There are some experimental complications in determining the exact band gap, including the tails of the optical spectra that can extend to several tenths of an eV. The calculated effective masses for the n-type carriers around the conduction band edge are $m_{n||} = 1.1 \pm 0.2 m_0$ and $m_{n\perp} = 0.30 \pm 0.03 m_0$. Here, the notations $||$ and \perp refer to the directions parallel and perpendicular to the Δ_1 band, respectively. Our calculated effective masses are very close to the reported experimental results of $m_{n||} = 1.4 m_0$ and $m_{n\perp} = 0.36 m_0$. There is a strong nonparabolic dispersion of the Δ_1 band around the conduction-band minimum. This leads to a relatively larger uncertainty in obtaining the effective mass and is also part of the reason for the differences in calculations of the effective masses for $m_{n||}$, using different methods.

We listed in Table 1 some calculated interband-transition energies at selected critical points. The calculated valence-band width of 21.35 eV is in an excellent agreement with the experimental value of 21 ± 1 eV. The calculated transition energies agree very well with experimental results.

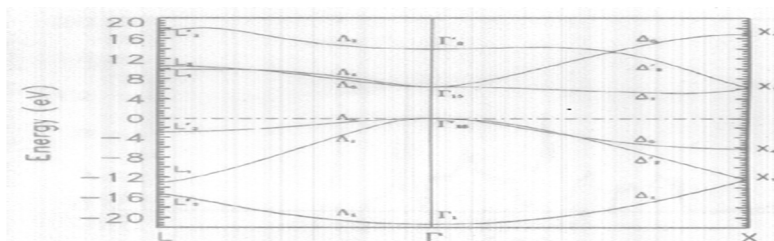


Fig. 1: The calculated electron band structure of diamond (C) along the symmetry direction Λ and Δ , as obtained with the optimal basis set of the BZW procedure.

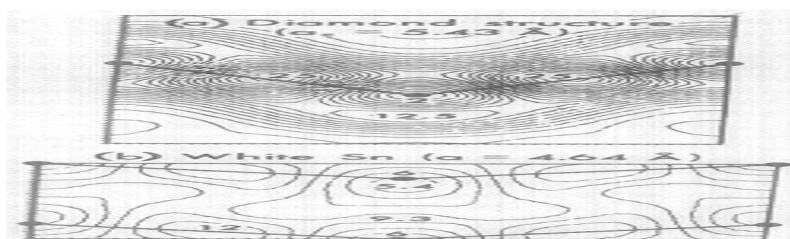


Fig.-2. The total valence charge density contours of bulk Si for (a) the diamond structure at $a_c = 5.43$ Å, and (b) the white Sn structure at $a = 4.64$ Å.

Table 1. Comparison of the calculated interband-transition energies (in eV) for silicon (Si) with experimental results.

R_g	1.02	1.14 ^a , 1.17 ^b
$\Gamma_{1v} \rightarrow \Gamma'_{25v}$	12.1	12.5±0.6 ^b
$\Gamma'_{25v} \rightarrow \Gamma_{15c}$	2.68	3.0 ^c , 3.4 ^d
$\Gamma'_{25v} \rightarrow \Gamma'_{2c}$	3.19	
$X_{4v} \rightarrow \Gamma'_{25v}$	2.93	2.9 ^e , 3.3±0.2 ^f
$\Gamma'_{25v} \rightarrow X_{1c}$	1.26	1.3 ^b
$L'_{2v} \rightarrow \Gamma'_{25v}$	9.80	9.3±0.4 ^b
$L_{1v} \rightarrow \Gamma'_{25v}$	7.04	6.8±0.2 ^b
$L'_{3v} \rightarrow \Gamma'_{25v}$	1.36	1.2±0.2 ^b
$\Gamma'_{25v} \rightarrow L_{1c}$	1.66	1.65 ^g , 2.1 ^h
$\Gamma'_{25v} \rightarrow L_{3c}$	3.78	3.9±0.1 ^b , 4.15±0.01 ⁱ
$L'_{3v} \rightarrow L_{1c}$	3.0	3.2±0.2 ^b , 3.45 ^d
$L'_{3v} \rightarrow L_{3c}$	5.14	5.1±0.2 ^b , 5.5 ^d

These calculated effective masses are very close to the experimental values of $m_{nt} = 0.19m_0$ and $m_{ni} = 0.98m_0$. The good agreements between the calculated effective mass and the band gap, with corresponding experimental results, indicate that the lowest conduction band in Fig. 1 is reasonably reliable. Table 1 shows the calculated interband-transition energies, along with experimental results, at selected critical points in the optical spectrum. In this table the indices v and c refer to the valence and conduction bands, respectively. The calculated optical transitions agrees well with experimental results. This agreement is particularly significant in light of difficulties in analyzing experimental data, including the effect of lifetime corrections. Values for the diamond, fcc, and bcc structures are quoted from ref. 20 [$\gamma(\text{diamond})$ can be calculated from the relation $\gamma(\text{diamond}) = \gamma(\text{fcc}) + \gamma(\text{bcc}) - \gamma(\text{sc})$ for the same a_c], and values for the hcp, white Sn, and the slab structure are calculated analytically.

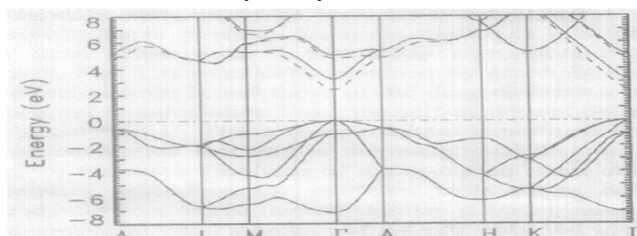


Fig. 3. Comparison of the results of calculation

V. CONCLUSIONS

We believe this is the most comprehensive study to date for wurtzite crystals and the results obtained are in good agreement with experimental data. The band structures obtained are more accurate than earlier calculation using a semi-*ab initio* OLCAO approach. With the exception of AlN and GaN, experimental results on other wurtzite crystals appear to be very limited. Our first-principles calculation will certainly be very useful for the interpretation of future experiments. We intend to use the present results on ideal perfect crystals as a starting point for future studies on more realistic systems involving defects, impurities, interfaces, and superlattice structures of these crystals. Also of interest is the change of electronic structures and optical properties of W crystals under pressure.

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