

A Mathematical Solution to the Theoretical Band Gap Underestimation: *Predictive Calculations of Properties of Semiconductors*

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OUTLINE

I. INTRODUCTION: A brief Historical Overview of Electronic Property Calculations and Related Approximations and Limitations

II. THE BAND GAP UNDERESTIMATION: Serious discrepancies between calculated and measured values of energy & band gaps of materials & between Schemes aimed at resolving the problem

III. MOTIVATIONS: To resolve the above discrepancies and to predict, *from first principle calculations*, E-gaps and other electronic properties of materials

IV. METHOD: THE BAGAYOKO, ZHAO, AND WILLIAMS (BZW) METHOD

General: LCAO (LCGO) and DFT & particularly LDA Potentials

Specific: the Bagayoko, Zhao, and Williams (**BZW**) Method

J. Phys. Condens. Matter 10, 5645, 1998 for BaTiO₃

Phys. Rev. B60, 1563, 1999 - - Diamond, Si, and GaN

V. SOME ILLUSTRATIVE RESULTS: For GaN, Si, Diamond, SWCNT, SiC (3C & 4H), ZnO, ZnSe, AlN, Si₃N₄, Ge, InN, InAs, GaAs, AlAs (E(**k**), Gaps, Effective Masses, etc.)

VI. CONCLUSION: DFT and LDA potentials, contrary to some previous and understandable beliefs, correctly describe electronic and related properties of semiconductors, including band gaps, if one implements the BZW Method.

I. HISTORICAL OVERVIEW: THE FUNDAMENTAL EQUATION

Note well that these equations are non-relativistic – hence, they are not the ultimate equations. They are approximations, the best we know!

$$\left[-\frac{1}{2} \sum \nabla_i^2 - \sum_{A,i} \frac{Z_A}{r_{Ai}} + \sum_{A>B} \frac{Z_A Z_B}{R_{AB}} + \sum_{i>j} \frac{1}{r_{ij}} \right] \psi(\vec{r}, \vec{R}) = E_{el} \psi(\vec{r}, \vec{R})$$

The Born-Oppenheimer approximation applied to the above equation leads to the following (note the absence of R in “Hamiltonian” and in the wave function):

$$\left[-\frac{1}{2} \sum \nabla_i^2 - \sum_{A,i} \frac{Z_A}{r_{Ai}} + \sum_{i>j} \frac{1}{r_{ij}} \right] \psi(\vec{r}) = E_{el} \psi(\vec{r})$$

HISTORICAL OVERVIEW (early 1930s): THE HARTREE FOCK EQUATIONS

$$\left[-\frac{1}{2} \nabla^2 - \sum_A \frac{Z_A}{|\vec{r} - \vec{R}_A|} + \sum_{i=1}^N \sum_{\sigma'} \int \phi_i^*(\vec{r}' \sigma') \frac{1}{|\vec{r} - \vec{r}'|} \phi_i(\vec{r}' \sigma') d^3 \vec{r}' \right] \phi_k(\vec{r} \sigma) - \sum_{i=1}^N \sum_{\sigma'} \int \phi_i^*(\vec{r}' \sigma') \frac{1}{|\vec{r} - \vec{r}'|} \phi_i(\vec{r} \sigma) \phi_k(\vec{r}' \sigma') d^3 \vec{r}' = \varepsilon_k \phi_k(\vec{r} \sigma).$$

These non-linear, integro-differential equations embed the following approximations [not eigenvalue equations of the form $H\psi = \varepsilon\psi$]

- Neglect of relativistic effects
- Born-Oppenheimer approximation (no nuclear motion, decoupling of phonon & electronic properties)
- Single Slater determinant assumed sufficient (see Configuration Interactions – CI)
- An electron is assumed to move in the means fields created by the others
- The central field approximation (in practice)

HISTORICAL OVERVIEW: DENSITY FUNCTIONAL EQUATIONS – LOCAL DENSITY APPROXIMATION (LDA) - Starting in 1964 & 1965

EQUATION 1 (Only for the ground state)

$$\left[-\frac{1}{2} \nabla^2 + V(\vec{r}) + \int \frac{n(\vec{r}')}{|\vec{r} - \vec{r}'|} d\vec{r}' + V_{xc}(n(\vec{r})) \right] \psi_i(\vec{r}) = \varepsilon_i \psi_i(\vec{r})$$

Equation 2 (Sum over occupied states only)

$$n(\vec{r}) = \sum^N \psi^*(\vec{r}) \psi(\vec{r}) \quad \text{Sum over occupied states only}$$

II. THE BAND GAP UNDERESTIMATION: DEFINITION OF TERMS

In finite systems, like atoms, molecules, clusters, etc., the energy levels occupied by electrons are discrete. For the hydrogen atom, they are given by the negative of a constant over n^2 , where n is the principal quantum number.

The energy gap of a discrete system is the lowest, unoccupied energy value minus the highest occupied energy value.

In crystalline solids, by virtue of the Bloch theorem, the energy levels of electrons are functions of a continuous parameter \vec{k} . Hence, they form bands.

The band gap for solids is the lowest, unoccupied energy value ($E_{\min,c}$) minus the highest occupied energy value ($E_{\max,v}$). It can be a **direct** gap (If $E_{\min,c}$ and $E_{\max,v}$ occur at the same \vec{k}), it is otherwise **indirect**.

Metals are the only materials with no band gap. Finite systems (atoms, etc.), semiconductors, and insulators have energy or band gaps that are important for most of their electronic properties and related properties (i.e., optical ones).

THE BAND GAP UNDERESTIMATION (1a)

Illustrative Discrepancies between the Measured and Calculated Band Gaps of ZnO in the Wurtzite Structure.

EXP1	EXP2	LDA 1	LDA2	LDA3	LDA4	GW1	GW2	HF
3.44 eV	3.30 eV	0.78 eV	1.15 eV	2.26 eV	0.77 eV	2.44 eV	4.28 eV	8.61 eV*
Low T	Room T	0 T	0 T	0 T	0 T	0 T	0 T	0 T

Exp: Experiment, **LDA:** Local Density Approximation, **GW:** Green Function and Screened Coulomb Approximation; **HF:** Hartree Fock Method

LDA-BZW value of the band gap of ZnO: 3.2 eV in excellent agreement with exp.

THE BAND GAP UNDERESTIMATION (1b)

Table I. Comparison of theoretical and experimental band gaps of **AIs** in eV.

	EXP1 T=4K	EXP2 T=295K	LDA1 (PAW)	LDA2 (PP)	LDA3 (PP)	LDA4 (FLAPW)	GW1 (PAW)	GW2 (PP)	GW3 (QP)	LDF (MB semi- ab-initio OLCAO)	TBM1	TBM2
E_g^X	2.23	2.16	1.32	1.20	1.44	1.36	1.57	2.08	2.09	2.37	2.21	2.14
E_g^Γ	3.13	2.98	1.94	1.77	2.35	1.95	2.72	2.75	3.26	2.79	2.81	3.00
E_g^L		2.36	2.06	1.89	2.12	2.07	2.73	2.79	3.03	2.81	2.48	2.31

- **Illustrative Discrepancies Between Measured Values and Calculated Values**
- **Those band gaps agreeing with exp. were generated not from ab-initio, self-consistent calculations, but from fitting-associated procedures**

Band gaps: indirect E_g^X ($\Gamma15v - X1c$), direct E_g^Γ ($\Gamma15v - \Gamma1c$), indirect E_g^L ($\Gamma15v - L1c$)

EXP1: experiment 1; Excitonic gap, Photoluminescence

EXP2: experiment 2; Transport

FLAPW: Self-consistent full-potential linearized-augmented-plane-wave

GW: Green Function and Screened Coulomb Approximation

LDA: Local Density Approximation

PP: Pseudopotential method

QP: Quasiparticle

PAW: Projector-augmented-wave

LDF: Local Density Function

TBM: Tight-binding model

THE BAND GAP UNDERESTIMATION (1c)

Illustrative Discrepancies Between the Theoretical Values of the Band Gap of Cubic Indium Nitride (**c-InN**)

Potential	Computational Method	a (Å)	B(GPa)	E _g (eV)
Local Density Approximation (LDA) Potentials	Pseudopotential Method (PP)	4.95	145	-0.36^a, -0.40^b
		5.004	140	-0.35^e, -0.18^g
	LAPW	4.94	145	
	Full Potential LAPW	5.03	138	-0.11^h & -0.48^h
	Full Potential LMTO			-0.4ⁱ
4.92		139 ^j		
	Atomic Sphere Approximation			-0.1ⁱ, +0.02 and +0.08^k
Generalized gradient approximation (GGA)	PP	5.06 & 5.109	120 ^c 118	-0.55^b
LDA plus SIC		5.05 ^d		+0.43^a
QP Calculation	PP			+0.52^a

PLEASE SEE MORE ON THE NEXT PAGE

THE BAND GAP UNDERESTIMATION (1c')

Illustrative Discrepancies Between the Theoretical Values
of the Band Gap of Cubic Indium Nitride (c-InN)

Potential	Computational Method	a (Angstroms)	B(GPa)	E _g (eV)
QP+SIC	PP			+1.31 ^a
DFT Exact Exchange				+1.4 ^g
DFT, SX	ASA			+1.3 ⁱ
Estimate of the bulk modulus of c-InN			137 ^l	
Empirical Pseudopotential Calculations (EMP)				+0.592 ^m
Experimental: Measured lattice constants		4.97 ± 0.01 ⁿ 4.98 ^o & 4.986 ^p		

NOTE: Other LDA Values of E_g: from -0.40 to + 0.08 for C-InN

QP, EXX, SX Values: From +1.3 to 1.4 eV

LDA-BZW Values: **0.65 eV** a = **5.017** Angstroms

Experimental Values: **0.61 eV** and a = **5.01 +/- 0.01** Angstroms

THE BAND GAP UNDERESTIMATION (1d)

Illustrative Discrepancies Between (a) Measured Values and (b) Calculated Values, and (c) Measured and Calculated Values of the Band Gap of Wurtzite Indium Nitride (w-InN).

	EXP Group 1	EXP Group 2	LDA PP	LDA FP-LMTO	GGA PP	GWA or QP (pp)
w-InN →	1.9-2.0 eV	0.7-1.0 eV	-0.4 to -0.2 eV	0.2 to 0.43 eV	-0.37 eV	.74 &.5 eV
c-InN →	Not Available	Not Available	-0.18 to -0.40 eV	-0.1 eV	-0.55 eV	0.52 &1.31

NOTE: LDA-BZW RESULTS: **0.88 eV**, exactly as experiment with same charge carrier concentration (Burstein-Moss Effect)

Exp: Experiment (group 1 before 2000, Group 2 after 2000);

LDA: Local Density Approximation;

GWA: Green Function and Screened Coulomb Approximation;

PP: Pseudopotential Method;

FP-LMTO: Full potential linear muffin tin orbital method

THE BAND GAP UNDERESTIMATION (2a): Explanations of the sources of discrepancies

In addition to the approximations inherent to the above discussed equations, theorists put forward explanations of the sources of the discrepancies for DFT calculations:

- DFT is reported to contain an error stemming for **having an electron interact** with itself (Perdew and Zunger, 1981)—They devised a ***self-interaction correction*** .
- **Derivative discontinuities** (John Perdew et al.1982) of the exchange correlation energy (Exc) in DFT (i.e., discontinuity of V_{xc}).
- **Derivative discontinuities** of Exc and of the of the kinetic energy (Ks) of non-interacting particles as given in the Kohn-Sham equation (Perdew and Levy, 1983). They assert that the discontinuity of V_{xc} is non-zero in semiconductors. **(We could not find a proof of this assertion.)**
- **Derivative discontinuities** of V_{xc} and of Ks (Sham and Shlüter, 1983). They state that they do not know if the discontinuity of V_{xc} is non-zero. They do not know the value of the discontinuity and do not claim it to be non-zero.

THE BAND GAP CATASTROPHE (2b): The proliferation of schemes (mostly ad hoc)

As we stated in some J. Appl. Phys. publications, the continuing proliferation of schemes purporting to resolve the band gap problem resembles that of epicycles for the Ptolemaic “Earth” system. (Well known for ~2000 years!)

It seems that by citing the above papers, authors can do practically anything and get it published: for them “**It is well known that density functional theory underestimates the band gap of materials.**” This practice continues even though a mathematical solution to the problem was provided by BZW in 1998 and 1999 – **This situation and the gap problem constitute a catastrophe.**

Some articles at the end of this presentation describe some of these schemes that include:

GW Approximation (mostly ab-initio)

SIC

LDA +C

EXX

TDDFT (for excited states, ~ ab-initio)

Hybrid Functionals (Chemistry), **Scissors approximation**, **gKS**, and more

GGA and **meta-GGA** (mostly ab-initio)

LDA + Wigner Interpolation

LDA + U (U is from Hubbard theory)

sX (X screened)

WDA (weighted DF Approximation)

III. MOTIVATIONS

The key motivation for our work was simply to resolve the above described energy gap and band gap problems and related use of EXTENSIVE talents and times to produce ad-hoc results with little or no predictive value.

The quintessential importance of correct **energy gaps**, correct **effective masses**, and of correct **optical**, and **related properties** of materials simply warrants any effort to get these quantities from first-principle calculations – TO USHER IN AN ERA OF TRUE PREDICTIVE CALCULATIONS OF PROPERTIES OF MATERIALS (ATOMS, MOLECULES, CLUSTERS, SEMICONDUCTORS, INSULATORS, & NUCLEI).

An added motivation was that, **at the nanoscale**, quantum effects are both ubiquitous and non-negligible. Hence, getting these effects correctly was deemed to be pivotal for further progress.

IV. METHOD

A. THE LCAO (LCGO) FORMALISM

THE EIGENVALUE EQUATION, $H\psi = E\psi$, IS SOLVED SELF-CONSISTENTLY BY TAKING

$$\Psi = \sum_{i=1}^N a_i \Phi_i, i = 1, N$$

The Φ_i are obtained from calculations the atomic or ionic species that are present in the system (including radial & angular features)

We employed **Gaussian orbitals** (LCGO) for the radial functions involved in the orbitals.

B. THE POTENTIAL

We utilized the local density functional potential of Ceperley and Alder as parameterized by Vosko, Wilk, and Nusair (VWN).

This choice is justified, for semiconductors, due to the utilization of the BZW procedure that ends the **confounding between LDA limitations and other problems.**

IV. METHOD (cont'd)

C.1. THE RAYLEIGH THEOREM

$$\text{Let } H\Psi = E\Psi$$

The linear combination of atomic orbital (LCAO) method leads to:

$$\Psi = \sum_{i=1}^N a_i \Phi_i, \quad i = 1, N$$

Let E_i^N be the **self-consistent** eigenvalues, **ordered from the lowest E_1^N to the highest E_N^N**

Let the above equation be solved with $(N+1)$ orbitals obtained by adding one orbital to the previous set of N orbitals. And let be the new self-consistent

eigenvalues, $E_i^{(N+1)}$, be ordered from the lowest, E_1^{N+1} , to the highest. These eigenvalues are obtained with the larger basis set of $(N+1)$ orbitals.

Then, by the Rayleigh Theorem, $E_i^{(N+1)} \leq E_i^N$ for $i \leq N$.

IV. METHOD (cont'd)

C.2. THE BASIS SET AND VARIATIONAL EFFECT (source of gap probl.)

Using the Rayleigh theorem, BZW identified an **intrinsic, basis set and variational effect as follows.**

This effect is partly due to the fact that **only the wave functions of the occupied states** are including in the construction or reconstruction of the Hamiltonian (**i.e., the physics**) in going from one iteration to the next.

The potential is basically unchanged once the occupied energies converge (in values, branching, & curvatures). However, adding more orbitals will still lower some *unoccupied* levels by virtue of the Rayleigh theorem!

Such an “**extra**” lowering is the effect. It has been ascribed, for decades, to some limitations of LDA. *For details and illustrations, please see Inter. J. Quant. Chem., 17, 527, 1983; J. Phys. Condensed Matter 10, 5645, 1998; and Phys. Rev. B60, 1563, 1999.*

Explanation: *Researchers have been solving one equation out of a system of two coupled equations. Mathematically, that practice is simply incorrect.*

IV. METHOD (cont'd)

C.3. IMPLEMENTING THE BZW METHOD

Three or more self-consistent calculations are generally needed.

Calculation I employs the minimum basis set (MB Set) needed to just account for all the electrons.

In Calculation II, the MB set is augmented with orbital(s) representing the next, higher energy level(s) of the atomic (ionic) species in the system.

The **occupied energy levels** from Calculations I and II are compared (numerically and graphically).

Calculation III utilizes basis set II as augmented with orbital(s) representing the next, higher energy level(s) in the atomic (ionic) species.

The **occupied energy levels** of Calculations II and III are compared numerically and graphically.

This process continues until the occupied levels from Calculations N and (N+1) are found to be identical (within known errors, if any).

Then, Calculation N is our physics solution (No extras; see theorem).

V. ILLUSTRATIVE RESULTS

Figure 1: LCGO-LDA-BZW band structures of ZnO resulting from Calculation III (____) and Calculation IV (-----), with the Fermi levels from the two calculations superimposed. The calculated band gap of 3.47 eV is practically the same as the experimental one. The extra lowering of the conduction bands in Calculation IV seems from the Basis Set and Variational Effect. Larger basis sets lower them further, while the occupied energies remain unchanged (i.e., at their minima).

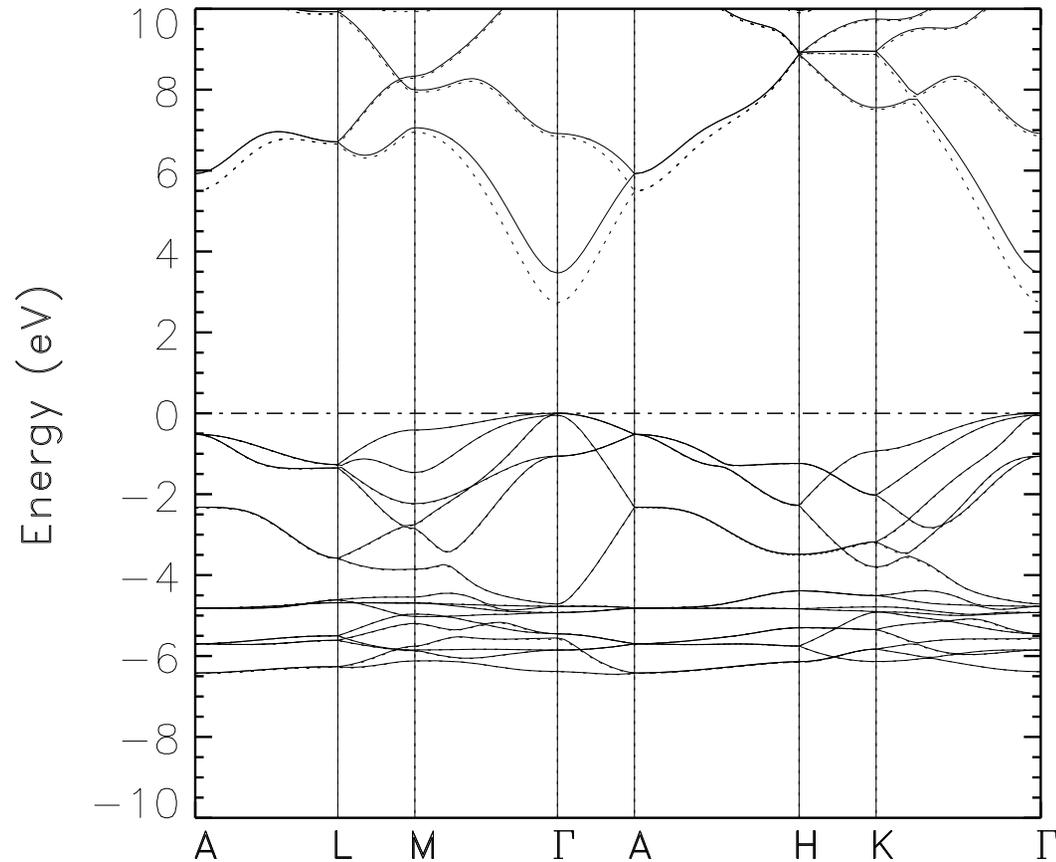


TABLE 2. Calculated Properties of Semiconductors versus Measured Values. [Computations done in accordance with the BZW procedure (i.e., optimal basis sets were obtained and utilized)]

Si	Calculation	Measurement	4H-SiC	Calculation	Measurement
Eg	1.02 eV	1.14, 1.17 eV	Eg	3.11 eV	3.2, 3.3 eV
W (valence)	12.1 eV	12.5 eV	$M_{n,\perp}^*$	0.41 $\pm 0.02 m_0$	0.42 m_0
M_{nt}^*	0.20 $\pm 0.03 m_0$	0.19 m_0	$M_{n,\parallel}^*$	0.31 $\pm 0.02 m_0$	0.33, 0.29 m_0
M_{nl}^*	0.93 $\pm 0.03 m_0$	0.98 m_0	$M_{MT\perp}^*$	0.62 $\pm 0.03 m_0$	0.58 $\pm 0.01 m_0$
			$M_{MK\perp}^*$	0.27 $\pm 0.02 m_0$	0.31 $\pm 0.01 m_0$
ZnO			c-Si₃N₄		
Eg	3.47 eV	3.44 eV	Eg	3.68 eV	(Not yet available)
AlN			ZnSe		
Eg	5.5-6.2 eV	3.9-6.2 eV	Eg	2.6-3.1 eV	2.8 eV
Carbon (8, 4) nanotube			Carbon (10, 0) nanotube		
Eg	0.90 eV		Eg	0.95 eV	

TABLE 3. Calculated Properties of Semiconductors versus Measured Values. [Computations done in accordance with the BZW procedure (i.e., optimal basis sets were obtained and utilized)]

<u>w-InN</u>	Prediction	Measurement	<u>c-InN</u>	Predictions	Measurement
Eg	0.88 eV	0.7-1.0 eV	Eg	0.65 eV	0.61 eV
			Latt. C.	a=5.017 Å	a=5.01±0.01 Å
<u>AlAs</u>	Calculation	Measurement	<u>InAs</u>	Calculation	Measurement
Eg	2.15 eV	2.23 eV	Eg	0.36 eV	0.35 eV

w-CdS: Calc. Eg = 2.47 Exp. 2.5 eV

zb-CdS: Calc. 2.39 eV Exp. 2.42 eV

Sodium Nitrite: Calc. Eg = 3.18 eV Exp. 3.14 – 3.22 eV

<u>TiO₂</u>	Calculation	Measurement	<u>Ge</u>	Calculation	Measurement
Eg	2.7 eV	3.0 eV	Eg	0.62	0.66-0.74
<u>GaAs</u>	Calculation	Measurement	<u>c-Si₃N₄</u>	Prediction	Measurement
Eg	1.24	~ 1.4 – 1.5 eV	Eg	3.68 eV	3.66 – 3.7 eV

Figure 1. Imaginary Part of the Dielectric Function – xy Component – for **w-InN**. **Experiment with $E_g < 1$ eV**

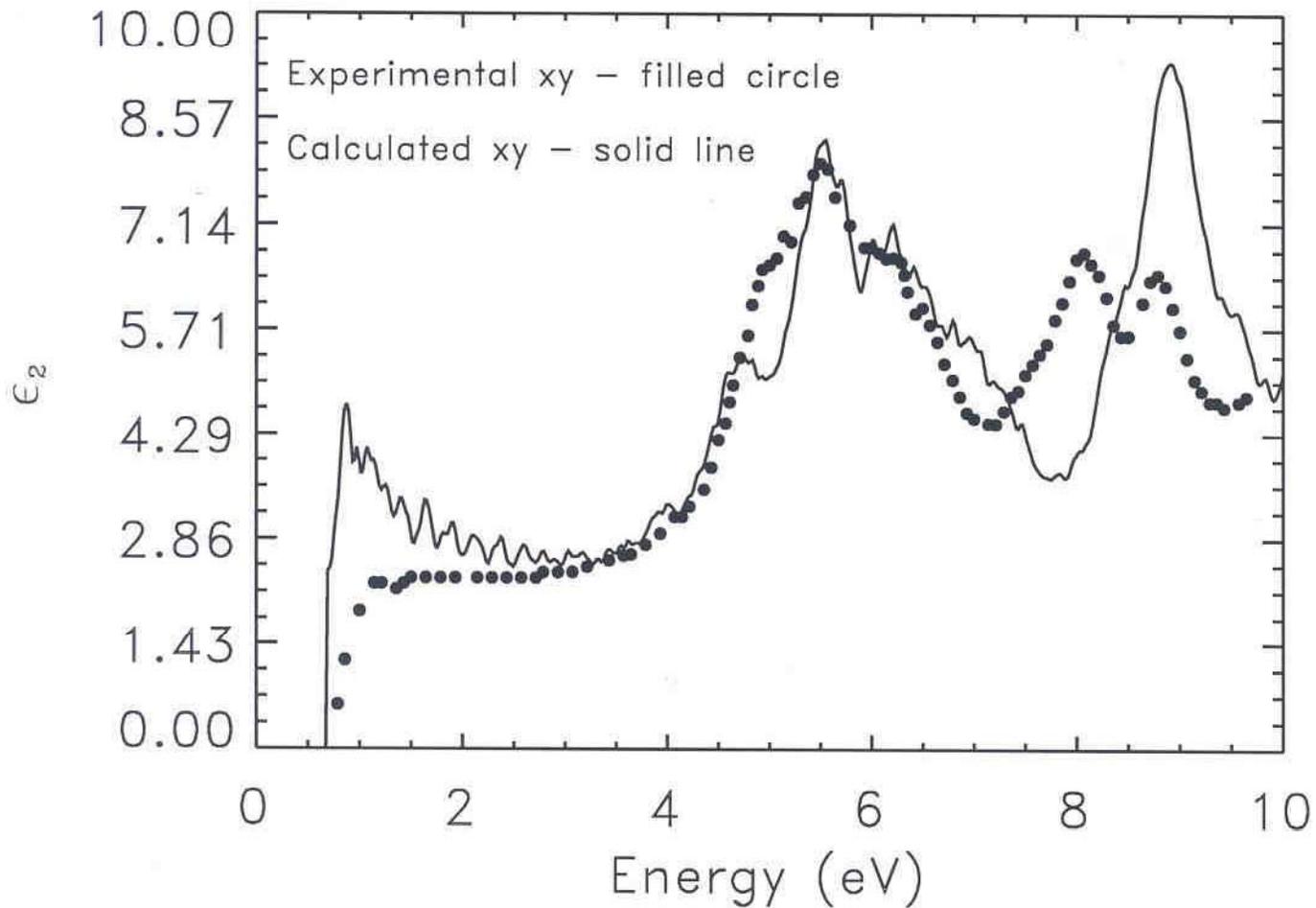


Figure 2. Imaginary Part of the Dielectric Function – ϵ_2 Component – for **w-InN**. **Experiment with $E_g < 1$ eV**

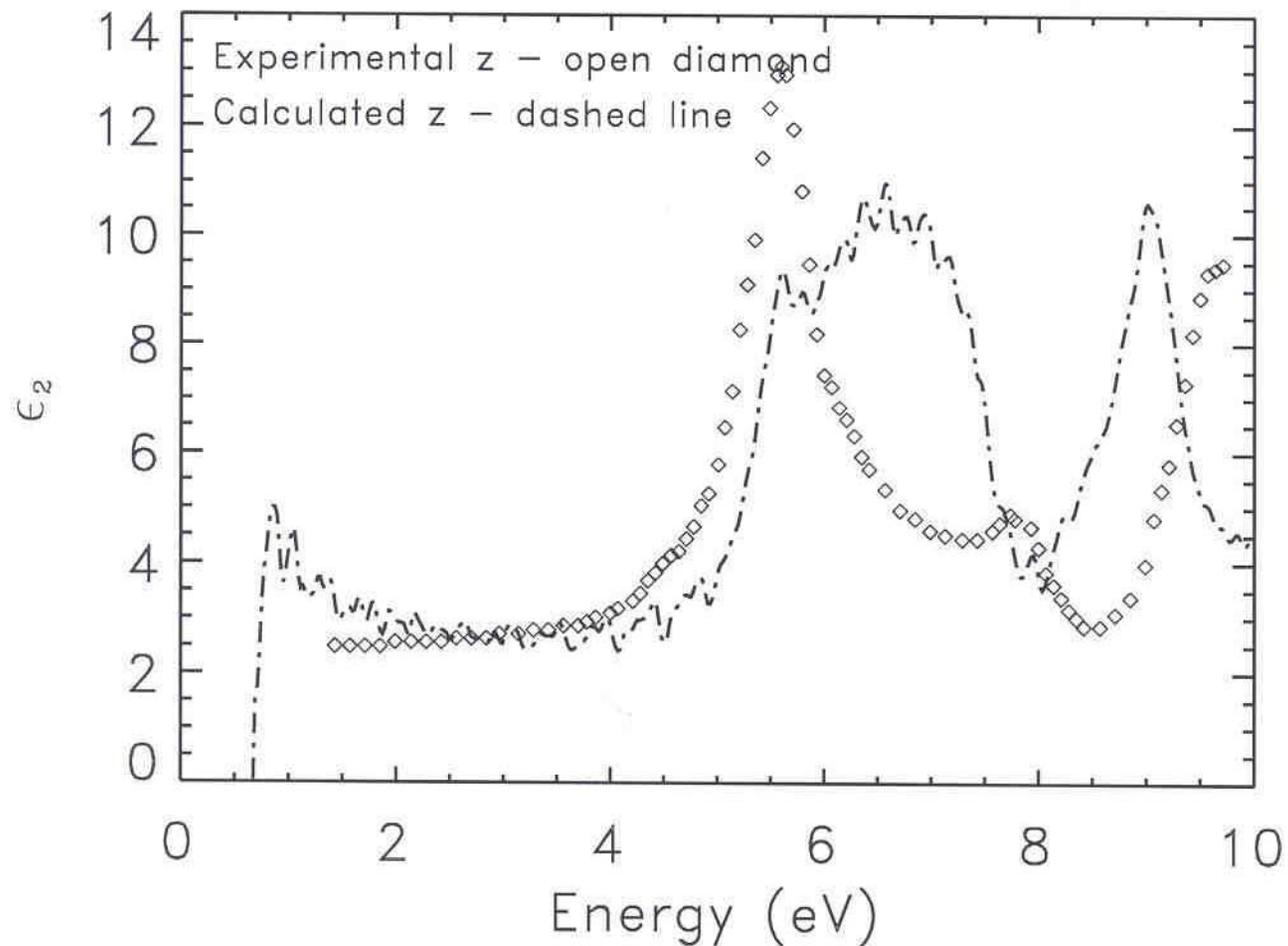


Figure 3. Real Part of the Dielectric Function – xy Component – for wurtzite InN (w-InN). **Experiment with $E_g < 1$ eV**

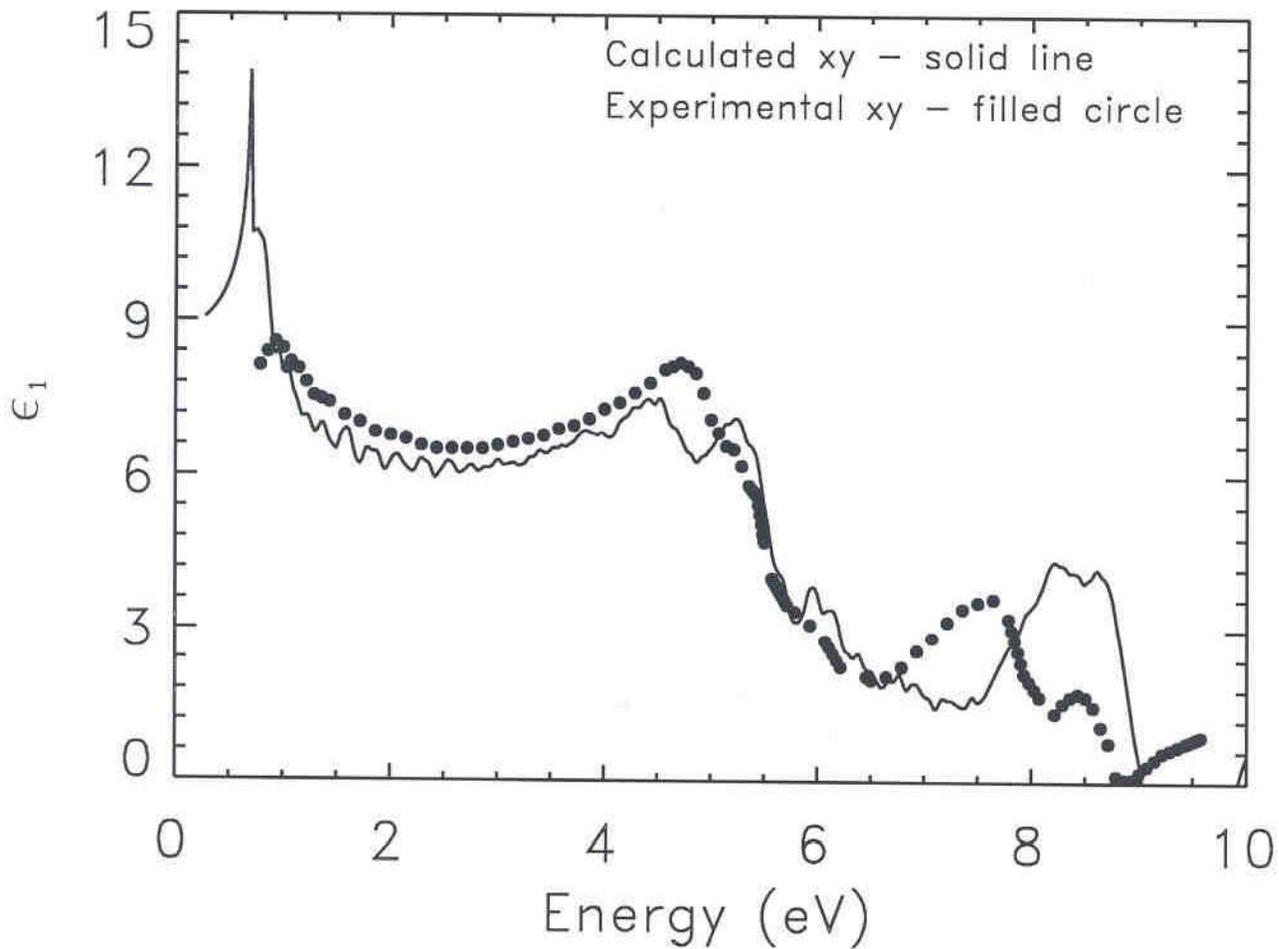
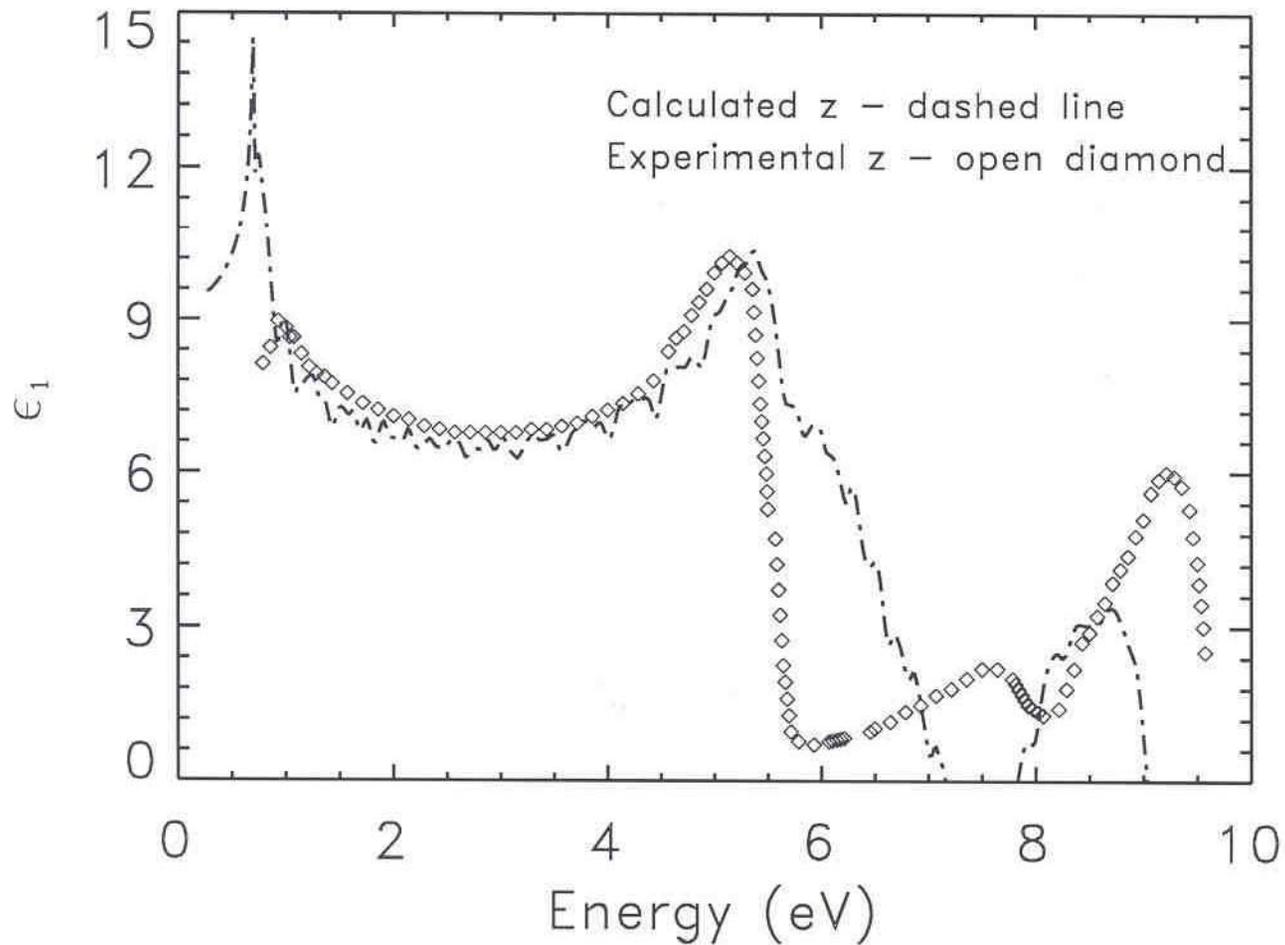


Figure 4. Real Part of the Dielectric Function – z Component – for wurtzite InN (w-InN). **Experiment with $E_g < 1$ eV**



VI. CONCLUSION

LDA-BZW calculations eliminate much of **the believed or perceived limitations** of density functional theory (DFT), with emphasis on the local density approximation (LDA).

Specifically, **low-energy conduction bands** and the **band gaps** are correctly described, mostly within experimental uncertainties, and **predicted by LDA-BZW calculations.**

The **gross discrepancies** illustrated and resolved above in case of w-InN have also been resolved for other materials including BaTiO₃, C, Si, GaN, ZnSe, AlN, c-Si₃N₄, Ge, InAs, GaAs, AlAs, TiO₂, and SWCNT, ZnO, etc.

The BZW method equally applies to the description **and prediction** of electronic and related properties of **atoms, molecules, clusters, semiconductors, and insulators**; [See **nuclei** (in the shell model).]

Measurements on c-InN and c-Si₃N₄ have confirmed the LDA-BZW predictions perfectly. The LDA-BZW correct values for effective masses and optical properties are not equaled by results from any other ab-initio method known to us.

VI. CONCLUSION (Cont'd)

IMPLICATIONS OF THIS CAPABILITY:

Molecular engineering (including the prediction or design of novel molecules, small or large, inorganic or organic)

Semiconductor engineering (including the prediction or design of materials with desired band gaps)

Enhancement of simulations (partly through accurate inter-atomic potential or empirical pseudopotential parameters derived from BZW results)

Theoretical exploration, using the nuclear shell model, of possibilities for gamma ray amplification by stimulated emission of radiation (graser).

Fundamental progress in the understanding of materials: i.e., a determination of the true capabilities and limitations of DFT and LDA and of schemes purporting to correct LDA or to go beyond DFT altogether.

THANK YOU VERY MUCH FOR YOUR ATTENTION

Annotated Bibliography

For a copy of this presentation or for one of any of the paper listed below, please send a request to D. Bagayoko at Bagayoko@aol.com

- "Contraction of Gaussian Basis Sets and the Total Energy of FCC Copper,"* D. Bagayoko, Inter. Jour. Quant. Chem. 17, 527 (1983). The Rayleigh theorem is enunciated and applied in this paper in connection with the explanation of the shifts (practically rigid) of the energy bands obtained with 35 contracted Gaussian orbitals as opposed to 75 single orbitals.
- "A Spurious Effect and LDA Prediction of the Correct Band Gap in BaTiO₃."* D. Bagayoko, G. L. Zhao, and Troy D. Williams. Bulletin, APS, Vol. 43, No. 1, p. 846, (1998). The first announcement and presentation of the BZW method.
- "Ab-initio Calculations of the Electronic Structure and Optical Properties of Ferroelectric Tetragonal BaTiO₃,"* Bagayoko, G. L. Zhao, J. D. Fan, and J. T. Wang, Journal of Physics: Condensed Matter, Vol. 10, No. 25, 5645 (June, 1998). This article did not just report the correct band gap of barium titanate, but also described correctly many measured optical properties. This paper is the first one where the BZW method is described (even though not named).
- "Local-Density-Functional Prediction of Electronic Properties of GaN, Si, C, and RuO₂,"* G. L. Zhao, D. Bagayoko, and T. D. Williams. Physical Review B 60, 1563, 1999. This paper showed, among other things, that the charge density and the Hamiltonian (i.e., the Physics) do not change for basis sets larger than the optimal basis set. Hence, the extra lowering of some unoccupied energies, when basis sets larger than the optimal one are utilized, is apparently not the manifestation of a physical interaction in a ground state theory.

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- “Electronic Structure and Charge Transfer in 3C- and 4H-SiC,”* G. L. Zhao and D. Bagayoko. New Journal of Physics (NJP), 2, 16.1-16-12, 2000. The BZW method successfully described the named materials within the local density approximation (LDA). This article is available free of charge at www.njp.org (search for Bagayoko or Zhao).
- “Effective masses of charge carriers in selected symmorphic and nonsymmorphic carbon nanotubes,”* G. L. Zhao, D. Bagayoko, and L. Yang, Phys. Rev. B 69, 245416, June 2004. As intimated in the conclusion of this presentation, the BZW method is believed to be indispensable in the theoretical description of nanomaterials for which (a) not only quantum effects are ubiquitous (a) but also are non-negligible.
- “Predictions of Electronic, Structural, and Elastic Properties of Cubic InN.”* D. Bagayoko, L. Franklin, and G. L. Zhao, Journal of Applied Physics, Vol. 96, No. 8, Pages 4297-4301, October 2004. As per the title of this article, the theoretical results therein are predictions of experimental values that have not yet been measured!

Annotated Bibliography (Cont'd)

“Density Functional Theory Band Gap of Wurtzite InN.” D. Bagayoko and Lashounda Franklin, Journal of Applied Physics 97, 123708, 2005.

“Density functional band gaps of AIAs.” H. Jin, G. L. Zhao, and D. Bagayoko, Phys. Rev. B 73, 245214(2006).

“Calculated Optical Properties of Wurtzite InN.” H. Jin, G. L. Zhao, and D. Bagayoko, J. Appl. Phys. 101, 033123 (2007). The excellent agreement with experiment, for energies up to 5.6 to 6 eV, denotes not only the correct description of the band gap, but also of the low-lying conduction bands! This conclusion also stems from agreements between our calculated optical transition energies and corresponding experimental ones for BaTiO₃ and other semiconductors.

Comment on *“Band structures and optical spectra of InN polymorphs: Influence of quasiparticle and excitonic effects.”* D. Bagayoko, L. Franklin, H. Jin, and G. L. Zhao, Phys. Rev. B 76, 037101 (2007).

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