

BZW Results for the Band Gaps of Bulk, Nanoscale, and Novel Semiconductors

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Abstract. We present new results of the application of the Bagayoko, Zhao, and Williams (BZW) method to the study of semiconductors and nanostructures. The 2000 Proceedings of the Malian Symposium of Applied Sciences [1] provide a detailed description of this relatively simple method that resolved a long-standing problem in theoretical solid state physics. These results, we hope, will encourage further application of the method whose predictive capabilities portend profound implications in the fundamental understanding of materials and in their technological applications.

Nous présentons des nouveaux résultats de l'application de la méthode de Bagayoko, Zhao, et Williams (BZW) à l'étude des semi-conducteurs et de nanostructures. Les Actes [1] du Symposium Malien des Sciences Appliquées, en 2000, fournissent une description détaillée de la méthode qui est relativement simple et qui a résolu un problème de longue date en physique théorique de l'état solide. Ces résultats, nous espérons, encourageront d'avantage l'utilisation cette méthode dont les capacités de prédiction ont des implications profondes dans la compréhension fondamentale de la matière et dans le domaine pratique de la technologie.

Key Words: energy bands, band gaps, effective masses, semiconductors, prediction

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Summary and Pertinent References

From the advent of quantum theory to very recently, calculated band gaps of semiconductors and of insulators grossly disagreed with experiment. Specifically, band gaps calculated with local density approximation (LDA) potentials were 30% to 50% smaller than experimental values. For most of the last 40 years, this disagreement between experiment and theory was ascribed to limitations of density functional theory (DFT) in general and the local density approximation (LDA) in particular. In 1998, we resolved this problem [2-5] by (a) identifying a basis set and

variational effect responsible for the discrepancies and (b) by developing and implementing a rigorous method for avoiding this effect in ab-initio calculations of properties of materials, with emphasis on non-metallic systems.

This brief article purports to present new results of the application of the BZW method. Consequently, we urge the reader to consult the above references. In particular, References 2, 3, and 4 provide a thorough description of the BZW method, *in English*, beginning with the Rayleigh theorem that led to the discovery of the basis set and variational effect. Additionally, these references provided correctly calculated band gaps of BaTiO₃ [2], diamond, silicon, GaN [3], ZnO, AlN, 3C-SiC, 4H-SiC, c-Si₃N₄ [4], and ZnSe [5]. We should note that our calculated band gap of 3.68 eV, for the newly discovered cubic phase of Si₃N₄ (c-Si₃N₄), is a *prediction*, given that no measurement of this gap existed at the time we first published our result. Reference 1, *in French*, also gives a full description of the method along with illustrative results.

The predictive capability of the BZW method, for the electronic and related properties of semiconductors, portends profound implications for device design and fabrication processes. In particular, BZW calculations can guide device fabrication processes due to their provision of correct band gaps for semiconductors. Further, they also predict correctly the locations and shapes of the lowest lying unoccupied energy levels or bands. In fact, the aforementioned basis set and variational effect primarily affects these levels or bands. Hence, BZW calculations also produce correct effective masses that are needed in the design of many semiconductor devices. Specifically, transport properties and the optical gain of semiconductors can be calculated using correct effective masses. *The prevalence and non-negligible nature of quantum properties of nanoscale materials further underscore the importance of the BZW method.* Indeed, the method is applicable not only to bulk and nanoscale materials, but also to the description or prediction of properties of atoms, molecules, and of novel materials that may be inorganic or biological. Its application to the nuclear shell model is expected to open the way to the identification of nuclei susceptible of enabling a population inversion. In other word, this particular application could introduce the gamma ray amplification by stimulated emission of radiation (graser) within the realm of possibilities.

With the above summary and specified references, we present below some results of the application of the BZW method. The results for the materials named above can be found in the identified references.

Selected Results

Table 1: The structural properties and band gaps of various carbon nanotubes (SWCNT), where L is the length of a unit cell in the direction of the nanotube axis; d_t is the diameter of the nanotube; N_a is the total number of atoms per unit cell; E_g is the band gap in electron volts (eV).

SWNT	L (°A)	d_t (°A)	N_a	E_g (eV)
(10, 0)	4.26	7.83	40	0.95
(13, 0)	4.26	10.18	52	0.75
(17, 0)	4.26	13.31	68	0.54
(22, 0)	4.26	17.23	88	0.44
(8, 4)	11.27	8.29	112	0.96

(10, 5)	11.27	10.36	140	0.74
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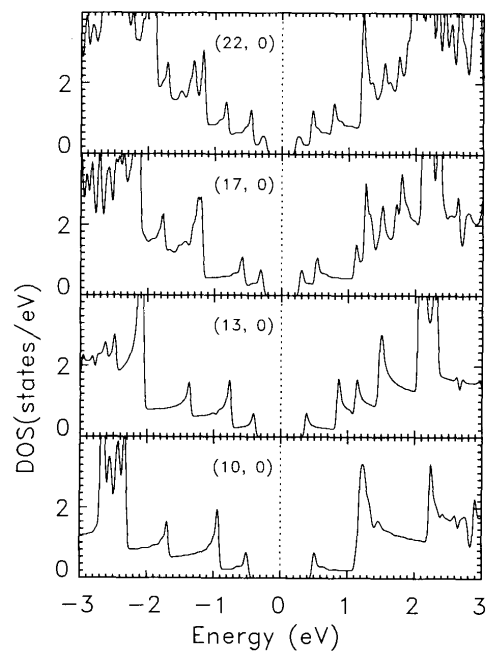


Figure 1. Total density of states (DOS) of selected carbon nanotubes as obtained with the BZW method. Zero is at the middle of the band gap, with the densities of the occupied states on the left and those of the unoccupied ones on the right.

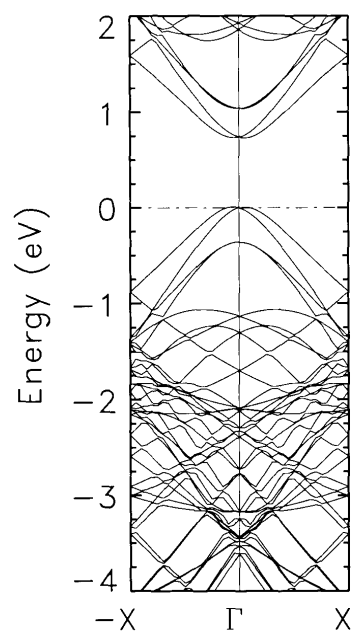


Figure 2. Electronic energy bands of (10,5) carbon nanotube as obtained with the BZW method. The Fermi level is set at zero.

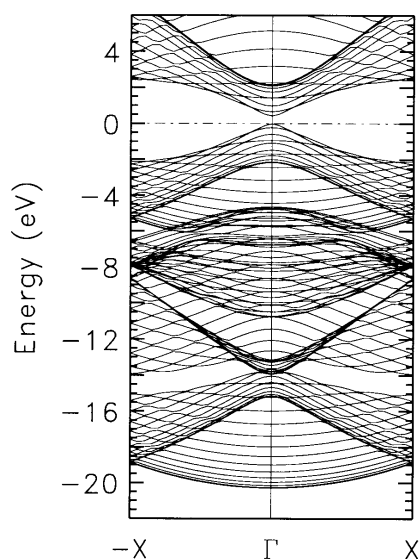


Figure 3. Electronic energy bands of carbon nanotube (22,0) as obtained with the BZW method. The Fermi level is set at zero.

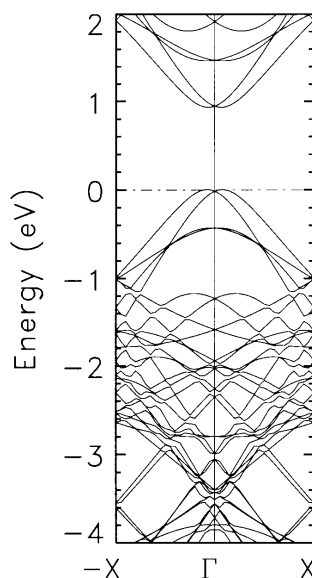


Figure 4. Electronic energy bands of (8,4) carbon nanotube as obtained with the BZW method. The Fermi level is set at zero.

Conclusion

We discussed the long-standing problem recently resolved by the Bagayoko, Zhao, and Williams (BZW) method, namely, the gross disagreement between theory and experiment for the band gaps of semiconductors and insulators. We guided the reader to the literature, in English and in French, where the method is described in detail. We presented some recent results for the band gaps of single-walled carbon nanotubes, and provided pertinent references with numerical results on other semiconductors. We underscored the utter importance of this very simple method that has profound implications not only for the fundamental understanding of materials, but also for their practical applications, including prospects for a gamma ray amplification by stimulated emission of radiation (graser). Given the possibility of performing the calculations on personal computer (PC), it is expected that some purposeful scientists will utilize the method not only to make contributions to science, but also to earn money. Indeed, in light of its predictive capabilities, the method permits the outright invention of novel materials (inorganic and organic) with desired and possibly exotic structures and properties.

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