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A Development of Self-Consistent Density Functional Program and Its Application to Electronic Structure Calculations of Semiconductors

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Abstract

A self-consistent density functional calculation program was developed and was applied to the electronic structure calculations of several narrow to wide gap semiconductors used in electronics and optoelectronics. Calculations showed the program can calculate the electronic structure of these semiconductors, accurately, from first principles. The program has published as a free ware and is going to be installed in K-supercomputer as a basic simulation software for electronics and material science.

1. Introduction

First principles density functional (DFT) method has been widely used in the semiconductor electronics community during the last two decades as a standard theoretical tool of investigating the electronic structure of solid state devices and materials. Enormous previous theoretical studies have successfully applied the method to the investigation of the structures and properties of devices and materials at the atomistic level. Examples include studies on high-k materials, high-k/semiconductor interface structures, defect and impurity states in gate insulators, Si oxidation processes, and electron transports in devices. Despite these brilliant successes, the DFT has a well-known severe problem: *i. e.* the band gap underestimation problem. Because the band gap of materials is a subject of major concern in solid state electronics, this problem imposes substantial limitations to the use of the DFT theory in the device and material study. In this study we have developed a self-consistent DFT (*sc*-DFT) program, to solve this problem. The program could calculate the electronic structure of several semiconductors very accurately, successfully solving the band gap underestimation problem from first principles.

2. Calculation Theory and Program Structure

The band gap underestimation by the DFT method is due to the residual self-Coulomb (SCI) interaction of DFT electrons [1]. The DFT Hamiltonian has, by construction, the SCI, and the SCI is exactly canceled out by the self-exchange interaction (SEI) of the electrons if the DFT exchange functional is exact. However, as the exact functional is unknown, approximate functionals such as those in local density approximation (LDA) or semi-local generalized-gradient approximation (GGA) are used in practical DFT calculations. The SEI by these approximate functionals is weak and insufficient in magnitude to cancel out the SCI, and the residual SCI remains as a result. The *sc*-DFT method accurately calculates the SEI by considering the screened Coulombic interaction of electrons, as the *GW* method does [2]. The exchange functional of the *sc*-DFT method v_x^{sc} is given by,

$$v_x^{sc} = \alpha v_x^{HF} + (1-\alpha) v_x^{GGA}, \quad (1)$$

where v_x^{HF} is the Hartree-Fock exchange and v_x^{GGA} is the exchange functional in the GGA. $\alpha = 1/\varepsilon$, and ε is electronic dielectric constant [3]. The electronic structure and ε are determined such that ε becomes self-consistent. Note that if α is constant and is set at 0.25, Eq. (1) gives the exchange functional of the PBE0 hybrid DFT method [4]. We developed a *sc*-DFT program based on *PHASE/0* and *UVSOR*, which are an electronic structure and an ε calculation program, respectively [5]. The flow-chart of the developed program is shown in Fig. 1. *UVSOR* is dynamically invoked by *PHASE/0* to calculate ε, in the calculation.

3. Results and Discussion.

Fig. 2 shows the *sc*-DFT calculation results of bulk Si. The calculation was started, using an ε of Si calculated with the PBE0 hybrid DFT method as the initial guess of ε. The calculation was converged at an ε of 11.5 and E_g of 1.09 eV after 7 iterations. These values are very close to experimental ε and E_g values of 1.11 and 11.7 eV, in contrast to a GGA calculation of Si which resulted in an E_g value of 0.6 eV. The band gap underestimation of the DFT was thus successfully remedied by the *sc*-DFT method in the Si case. Fig 3 shows the calculation results of InSb. The calculation is a stringent test of the *sc*-DFT method because InSb is a narrow band gap semiconductor and the GGA DFT method provides a zero band gap result. Although the calculation was stated, from a GGA electronic structure for InSb with a zero-band gap, it converged at an ε of 18.39 and an E_g of 014eV after 8 iterations. These calculated values are close to an ε of 17.13 and an E_g of 0.17eV. from experiments. The result indicates that the *sc*-DFT method is effective for calculating the electronic structure of narrow band gap semiconductors, for which the conventional DFT method provides zero-band gap results. The electronic structures of GaSb, Ge, GaAs, GaP, cubic SiC, cubic-cubic GaN, C (Diamond) and cubic-BN were similarly calculated by the *sc*-DFT method, and the calculated E_gs of these semiconductors and Si and InSb are plotted against their experimental E_gs in Fig. 4. E_gs of the semiconductors were also calculated by the GGA method for comparison. In contrast to the DFT method, which substantially underestimated

the E_gs of the semiconductors, the *sc*-DFT method could calculate the E_gs of them, almost quantitatively, working similar to the *GW* quasiparticle method in calculation performance. [2] The band underestimation problem of DFT was thus solved for narrow to wide E_g semiconductors of interest in electronics and optoelectronic by the developed *sc*-DFT program

3. Conclusion

A *sc*-DFT program was developed. The program has enabled the accurate electronic structure calculation of several semiconductors. The program has published has as a free ware at our web site [5] and is going to be installed in K-computer as a basic software for public use. We conclude that the developed program is a promising theoretical tool of studying solid state devices and materials from first principles.

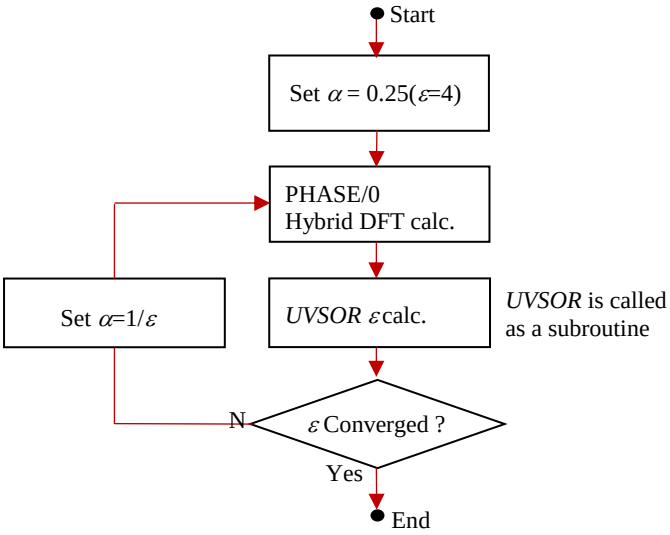

Fig. 1 Flow chart of the developed *sc*-DFT program. e and a are electronic dielectric constant and the weight of Hartree-Fock exchange in the exchange functional (see Eq. (1)).

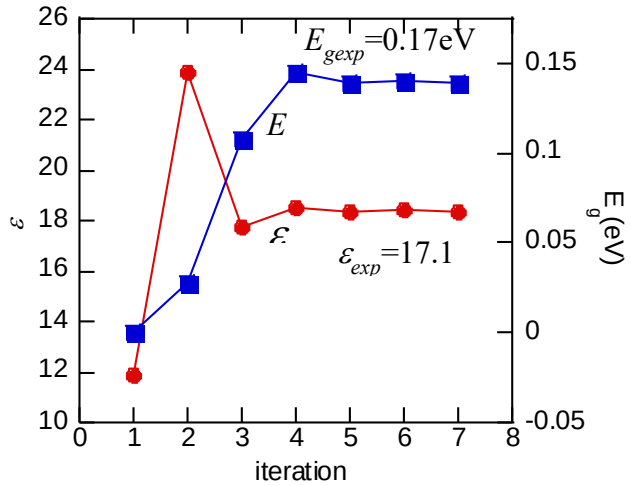

Fig. 3 Change of electronic dielectric constant ε and band gap E_g of InSb in the *sc*-DFT calculation. An ε and an E_g from experiments are shown for comparison.

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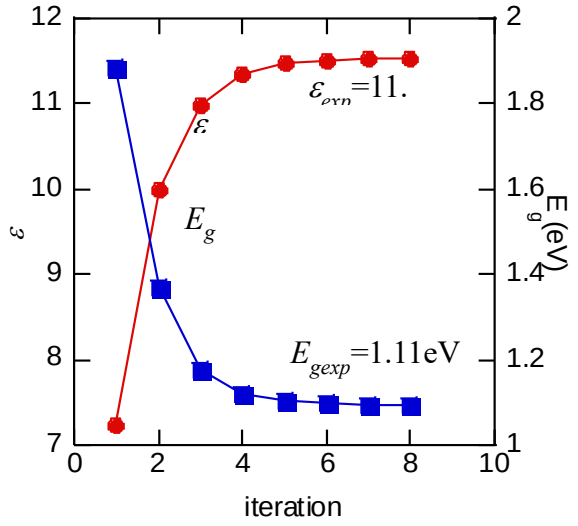

Fig. 2 Change of electronic dielectric constant *e* and band gap E_g of Si in the sc-DFT calculation, An *e* and Eg from experiments are shown

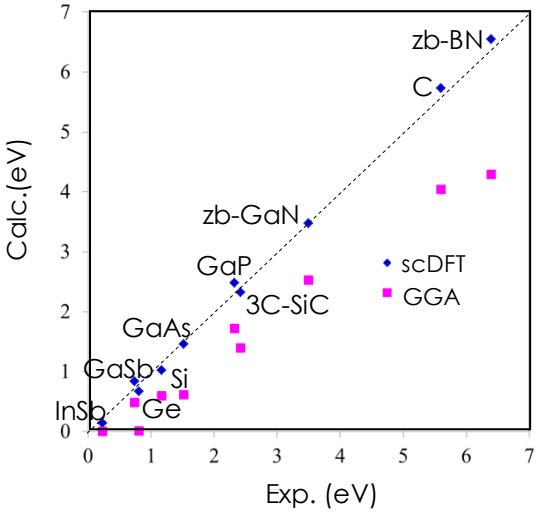

Fig. 4 Calculated versus experimental band gap of semiconductors. zb denotes zinc-blende(cubic) structure