Ab initio calculation and its application

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Semiconductors are widely used in our every-day life. Computers, TV, and various house ware contain semiconductor chips. Semiconductors attract more and more interest recently. Defects are common in semiconductors. Some of defects are intrinsic defects that are formed in the growth process. Some of the defects are external defects that are generated by radiation. Defects play important roles and affect various properties of semiconductors [1]. Defects can play a good role, n-doping and p-doping form the basics of computer chips. Defects can also play a bad role, they scatter electrons and generate unnecessary heat in computer chips. Understanding defects is fundamental to design small and fast chips.

Ab initio calculation is a useful tool to understand the defect physics. The most accurate calculations are based on ab initio calculations. There are various ab initio programs including VASP, Materials Studio, Wien2k, Abinit, Quantum Espresso, etc. The electronic structures as well as electronic density of states can be obtained by use of these software. Bonding properties can be analyzed from the charge distributions. Electronic spectrum can be computed. Defect formation energies can be calculated [2]. There are some ab initio programs that can handle phonons. MedeA software can draw phonon dispersion curves and phonon density of states. Phonopy software can also calculate similar properties and extract force constants from phonon calculations.

Ab initio calculation is time consuming. However recent development of computers make the huge calculations possible. Ab initio calculation is one of the theoretical tools. There exist various kinds of theoretical tools. Tight binding is still a simple and useful tool [3]. Many interesting physics were interpreted by use of the method. Tight binding force field can be used for empirical phonon calculations [3]. Nth order muffin-tin orbital (NMTO) method is a powerful tool to treat some strong correlation systems [4]. With development of GPU technology, molecular dynamics method is also a very attracted tool and can provide dynamical properties [5].

CdSe and CdTe are important in solar cells [6-8]. High frequency vibrational modes in CdSe is found experimentally [9]. In order to understand the origin of the modes. Ab initio calculations are desirable. Vacancies, interstitials are studied [9]. These simple defects cannot account for the high frequency modes. The authors propose OCd, that is oxygen atom occupy the Cd vacancy. This proposal cannot explain the high frequency modes [10]. There exist hydrogen related defects in CdSe [11]. The hydrogen impurities are from water contamination [12].

SiC is an important nuclear materials. It is a kind of wide band gap semiconductor. Magnetism is found in irradiated SiC. Detailed ab initio calculations confirm the origin of the magnetism is from divacancy in SiC [13]. Divacancy is not the only type of magnetic defects. There are many kinds of irradiated defects in SiC. Some of them are charged defects [14]. One kind of interstitial defect (IHe) can also be the magnetic defects [15]. There is a book that reviews the defect magnetism [16].

DNA conformation are important for their unique biological functions. Ab initio calculation is necessary to explore DNA conformations as well as DNA interactions [17]. The density of states of DNA and metal system can be calculated by ab initio program. The computed results are sufficient to recognize DNA bases [18]. Design of balanced dual ACE/NEP inhibitors is possible by ab initio calculations [19].

By use of ab initio calculations, most calculated properties are consistent with experiments. There are draw backs of the ab initio programs. Only systems with a few hundreds of atoms can be calculated by the program. So charged defects are difficult to be calculated because of long range Coulomb effect [14]. Band gap cannot be predicted correctly based on the ab initio program. G W is powerful to give correct band gap, however it is very time consuming. Ab initio program will continue to be developed. In the following decades, ab initio calculations will be more and more accurate in predicting various properties.
REFERENCES:

Wei Cheng was born in Jiaohe, Jilin province, China in July 1973. He received Ph.D. degree from the Institute of Theoretical Chemistry, Jilin University, China in 1999. From 1999 to 2003, he was an Assistant Professor at Institute of Low Energy Nuclear Physics, Beijing Normal University, China. In 2003, he joined School of Nuclear Science and Technology, Beijing Normal University, China, as an Associate Professor. He visited Illinois State University and University of California Berkeley, US, as a research scientist. He participated several programs in International Center for Theoretical Physics (ICTP) in Italy. His research interests include molecular dynamics simulation and ab initio calculation on defects in semiconductors.