Accurate electronic structure calculation on transition metal defects in silicon carbide polytypes

Viktor Ivády

Wigner Research Centre for Physics,
Hungarian Academy of Sciences,
PO Box 49, H-1525 Budapest, Hungary

Abstract

Relatively little is known about the complexty of point defects that may appear in different polytypes of a given crystal, which significantly influence their electrical and optical properties. Silicon carbide (SiC) is a prototype material for polytypism and many forms can be relatively easily fabricated.

SiC polytypes have a wide band gap where the electronic and optical properties can be significantly altered by introducing impurities. As a PhD student I have started to conduct research on characterizing transition metal defects in different polytypes of SiC by means of *ab initio* supercell calculations with the help of my supervisor. We collaborate tightly with the experimental group led by Professor Erik Janzén at Linköping University in Sweden. We run the *ab initio* codes at the supercomputer center installed at that campus.

The key issue in characterization of the metal impurities in SiC is to accurately calculate the electronic structure of these point defects which is a challenging task because of the strongly correlated d electrons together with the ordinary sp^3 bonds present in the system. So far I have applied a recently developed hybrid density functional in order to circumvent the well-known band gap error of (semi)local density functionals. My key results about the relative stabilities of different transition metal defects have been recently published in a Physical Review Letters paper. In order to calculate the charge transition levels and photoluminescence signals found by Janzén's group I would like to test different functionals beyond the applied hybrid density functional in order to be able to accurately predict the charge transition levels of selected transition metal defects. In addition, the optical signals would be determined by many-body perturbation theory based on the accurate ground state calculation.

The purpose of this short visit is to have an intense personal discussion with the experimental group at Linköping University in order to select the appropriate detected centers for these important case studies and to optimize the codes installed on the supercomputers at Linköping University mediated by the experts at the supercomputer center for efficient large scale calculations.

Report

The visit was successful and especially beneficial for me. Through the personal discussion with both experimental and theoretical researchers I could see different aspects of the issues of transitional metal related defects in SiC, and they exposed some very important questions. During some visit in the laboratories I could acquire profitable knowledge about experimental techniques. Thanks for this trip I could make progress in finding the appropriate theoretical description of these very important defects.

During the two weeks I was invited for two workshops where I could see the operation of a well organized research group was optimizing their present studies to achieve long-term purposes. Furthermore I could see the tight cooperation between experimental group and theoretical group at these meetings. I was invited for laboratory visits three times when the experimental issues of sample growing and measuring were introduced to me. I was an attendee at the seminar of an theoretical group is leaded by prof. Igor Abrikosov and I had a presentation about my previous work which was published in Physical Review Letters. The most profitable activities were the numerous discussions with experimental as wall as theoretical researchers. I had meetings with researchers from prof. Erik Janzén's group like Nguyen Tien Son, Ivan Ivanov and Andreas Gällström. We tried to find out the explanations of their recent experimental observations based on the results from our calculations. About theoretical questions I had a discussion with prof. Igor Abrikosov which was very useful for my present study.

The projected publications are related to the visit in Sweden: I carried out some calculations for Andreas Gällström about vanadium related defects in SiC to justify his assumptions which may appear in a joint publication. I had an accepted presentation at DPG conference in Berlin with the title: Accurate electronic structure calculation on transition metal defects in SiC by HSE06+U functional. With the same topic we are planning to write an article what we would like to publish in Physical Review Letters.

We want to continue this fruitful collaboration between the Hungarian group and the Swedish groups.