Semester Report-Semester I.
First principles investigation of solid state defects acting as quantum bits

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1 Introduction

Recently, quantum technology has become a leading driving source in science. Solid-state point defect based single photon sources and quantum bits are leading contenders for quantum technologies such as quantum computing, quantum communication and quantum sensing. After the success of the nitrogen-vacancy center in diamond acting as a qubit, the search for similar centers in other materials has been initiated mediated by first principles calculations [1, 2]. Most recently, defects in two-dimensional (2D) materials have been explored, acting as single photon sources or qubits, in particular, in hexagonal boron nitride [3].

I am studying point defects in 2D and 3D materials that may act as bright single photon source or qubit.

2 Research done this semester

I started the *ab initio* investigation of point defects in an exotic 2D material, namely, hexagonal or 2D silicon carbide (2D-SiC), which has recently been synthesized [4].

We applied the density functional theory (DFT) approach [5] with the projector augmented wave (PAW) method [6] in the Vienna Ab-initio Simulation Package (VASP) [7]. The exchange correlation functional of Heyd, Scuseria, and Ernzerhof (HSE06) was employed [8].

Table 1: Computed HF principal values (A_{xx}, A_{yy} and A_{zz}) in units of MHz for the atoms closest to the V_C-C_{Si}^{-} defect. The atoms included in the calculation are indicated in Fig. 1(b).

Atoms	A_{xx}	A_{yy}	A_{zz}
C_1	-2.86	-7.34	-1.69
C_2-C_3	-5.46	-3.9	-5.86
Si_1-Si_2	-1.46	4.52	-101.33

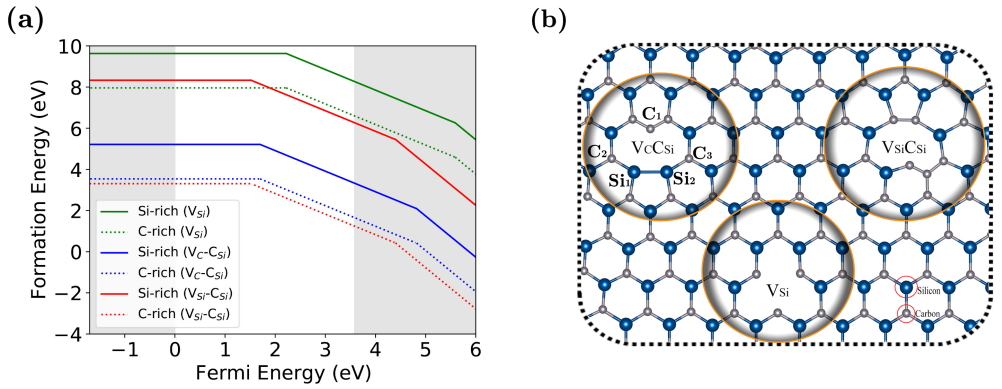

Figure 1: (a) Formation energy as a function of the Fermi level for the V_C-C_{Si}, V_{Si}-C_{Si} and V_{Si} defects, in Si-rich and C-rich growth conditions. (b) The atomic structures of V_{Si}, V_{Si}-C_{Si} and V_C-C_{Si} defects after optimization showing C_{2v}, C_s and C_{2v} point group symmetry, respectively. Si and C atoms are represented by blue and gray colors, respectively.

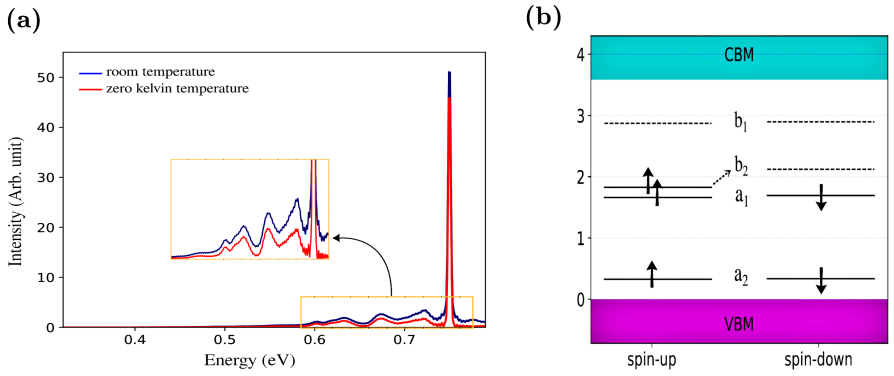

Figure 2: PL spectra for the electronic transitions in V_C-C_{Si}^-, with 52% of DW factor, at both room and zero-kelvin temperatures (a), and Electronic level diagrams for the ground states of V_C-C_{Si}^- defect(b).

The $8 \times 8 \times 1$ supercell was performed for all calculations using a Γ-point. We applied a vacuum region of 24Å in the z-direction for canceling all interactions between periodic images. The atomic positions were optimized to the point where the Hellman-Feynman forces acting on them were less than 0.01 eV/Å per atom, and a kinetic energy cutoff of 450 eV was used. Constrained DFT (CDFT) was employed to calculate the excited state [9].
The pristine 2D-SiC was optimized using HSE, which yields a lattice constant of $a = 3.07$ Å and Si-C bond length of 1.77 Å, while in the experimental measurement [4], these are 3.1 Å and 1.79 Å, respectively. Thus, the errors are less than 1.0%.
The point defects in 2D-SiC, namely a vacancy (V_{Si}) and two antisite vacancy pairs (V_C-C_{Si} and V_{Si}-C_{Si}), are examined (Fig. 1(b)) using ab-initio techniques for their potential as single-photon emitters (SPEs). We first calculated the formation energies and charge transition levels (Fig. 1(a)). All defects are only stable in the negative and neutral charge states. We find that the V_C-C_{Si} in the negative charge state is simultaneously stable and may have an infrared emission. Therefore, we carried out a detailed ab-initio characterization for this defect: ZPL energy is 0.59 eV, HR factor is 0.80, and DW factor is 44%. The radiative lifetime of the excited state of the defect is 155 ns. The PL spectrum at both

zero-kelvin and room temperature is plotted in Fig. 2(a). This defect has $S = 1/2$ spin state, so it is a paramagnetic defect. The calculated characteristic hyperfine constants are listed in Table 1, where the atom labels are depicted in Fig. 1(b).
We systematically studied the basic properties of Si-vacancy type defects in 2D-SiC. We found that the negatively charged V_C-C_{Si} defect has promising magneto-optical properties for realizing a single photon source with emission in the near-infrared region (see publication).

3 Publications

Vacancy-related color centers in two-dimensional silicon carbide monolayers
M. Mohseni, I. Abdolhosseini Sarsari, S. Karbasizadeh, Q. Hassanzada, T. Ala-Nissila, and A. Gali
https://doi.org/10.48550/arXiv.2208.09120

4 Conferences

Eötvös Loránd Fizikai Társulat, Magyar Fizikus Vándorgyűlés, VESZPRÉM
Pannon Egyetem, 21-24 of August, 2022.
The 19th of International Conference on Silicon Carbide and Related Materials(ICSCRM)
Davos, Switzerland, 11-16 of September, 2022

5 Studies

Physical materials science II. FIZ/1/016E
Introduction to quantum optics FIZ/3/029E

References

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[3] M. Fischer et al. “Controlled generation of luminescent centers in hexagonal boron nitride by irradiation engineering”. In: *Science Advances* 7 (8 Feb. 2021), pp. 7138–7155. ISSN: 23752548. DOI: 10.1126/SCIADV.ABE7138/SUPPL_FILE/ABE7138_SM.PDF. URL: https://www.science.org/doi/10.1126/sciadv.abe7138.

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[9] Adam Gali et al. "Theory of Spin-Conserving Excitation of the N-V-Center in Diamond". In: *Physical Review Letters* 103 (18 Oct. 2009), p. 186404. ISSN: 00319007. DOI: 10.1103/PHYSREVLETT.103.186404/FIGURES/2/MEDIUM. URL: https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.103.186404.