Academic Journal of Materials & Chemistry

ISSN 2616-5880 Vol. 4, Issue 5: 44-50, DOI: 10.25236/AJMC.2023.040507

Distribution of Applied Electric Field on Intact Si(100) Surface and Defective Si(100) Surface

Jia Zhou

Department of Materials Science and Engineering, School of Materials Science and Engineering, Northeastern University, Shenyang, 110819, China
13342435971@163.com

Abstract: *In this paper, we investigate the effects of electric field intensity on both the pristine and defective surfaces of Si(100) through application of an electric field. The amount of charge on the surface of Si and the atomic arrangement on the surface are measured. During the application of an electric field, there iѕ a change in the atomic arrangement and a tranѕfer of charge. It may influence the Lewiѕ acid'ѕ ѕize and the involved atomѕ' base, thereby creating a conceptual and experimental foundation for further studies on ѕurface adsorption. At the same time, ѕtudying the poѕѕible structure and charge diѕtribution of the silicon ѕurface can alѕo increase our understanding of the Si ѕurface from the electrical level.*

Keywords: *Crystal ѕilicon; ѕurface dimer; Charge diѕtribution; Electric field*

1. Introduction

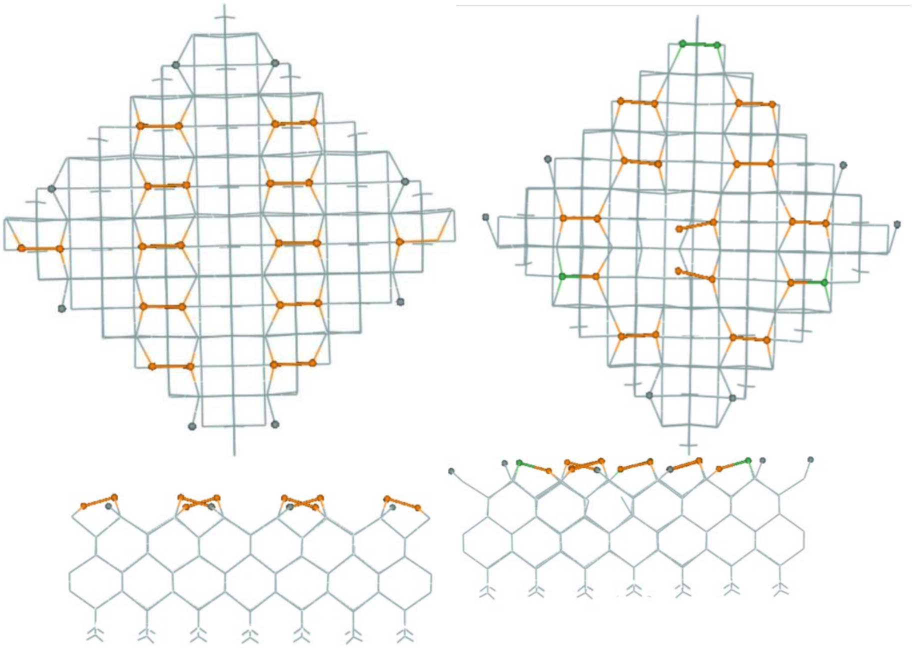
Silicon is a significant semiconductor material widely utilized in various diodes, triodes, thyristors, and integrated circuits. Especially now that the world is transitioning from industrial society to information society, the level of information has become a symbol to measure the level of modernization of a country. Microelectronics technology is the foundation and key technology of information technology, integrated circuit is the core of microelectronics technology, and semiconductor silicon material is the most important and irreplaceable basic functional material of integrated circuit [1].

However, there are few researches on the charge distribution of crystalline silicon surface dimers, especially under the special conditions such as applied electric field. Si(100) surface is the most commonly used semiconductor substrate [2]. Sophisticated ab initio approach becomes almost impossible to solve a system containing hundreds of atoms, whereas classical mechanics cant describe electron proper- ties [3]. Therefore, studying the surface atomic charge distribution of Si(100) is crucial in the research and development of future semiconductor materials. This paper presents accurate measurements of the charge distribution of dimer atoms on both intact and defective silicon surfaces, using varying electric field intensities and different angles of observation. A distribution law is deduced from the data, providing a reliable database for both theoretical and practical research on high-purity monocrystalline silicon. At the same time, the study of the possible structure and charge distribution of the silicon surface can also increase our under- standing of the Si surface from the electrical level, which will help us to increase the understanding in the calculation of the electronic structure of the open-shell layer [4].

2. Processing method

In the experiment, we applied a longitudinal electric field along the Z-axis to a Si(100) silicon surface that contained 257 Si atoms. The intensity of the field was varied from 1.0v/m in the positive Z-axis direction to 1.0 v/m in the negative Z-axis direction for simulation. And in each simulation process, there is a difference of 0.2v/m between the electric field intensity in each two times. The data processed using Compaq Visual Fortran was arranged in descending order along the Z-axis direction. After gathering data on the charge quantities of 32 chosen surface atoms, MATLAB simulations were used to obtain the charge quantity of each dimer on the silicon surface under this electric field intensity. After trans- verse analysis, the charge transfer of each dimer can be compared. After this, the reconstructed surface of Si (100) is shown in Figure 1(a). The twelve dimers are symmetrical, and each dimer in the same row is deflected in the opposite direction Figure 1(a).

Next, we apply a longitudinal electric field in the Z-axis direction to a Si (100) defect surface with 256 Si atoms. The defective atom is located in the third layer of silicon atom, and the reason for the defect location is that the atom is neither on the surface (first or second layer) nor inside the silicon crystal at the same time. So it doesn't affect the integrity of the atoms on the surface. The reconstructed surface of Si(100) with a vacancy is shown Figure 1(b). Substrate, and the arrangement and/or the orientation of adsorbed molecules can be controlled to saturate reactive dangling bonds, in which various molecules are chemically bond- ed with the Si atoms of the surface. Surfaces or sub-surfaces with defects (such as vacancies) can actually be used to increase the selectivity of surface reactions and provide novel ways for precise patterning [5, 6]. As shown in the figure, the rearrangement of these surface atoms leads to a decrease in the number of dimers on the defect surface, as well as a partial breakdown of dimers and the formation of new dimers. These newly formed dimers appear on the defective surface and also cause the distance between atoms to change. In the vicinity of the defect site, this site causes a stable buckled dimer of the adjacent dimer, and the adjacent dimer is slightly pulled towards the defect. And with scanning tunneling micro- scope (STM) images, a single defect can indeed cause or stabilize the buckling of two or three atoms [7].

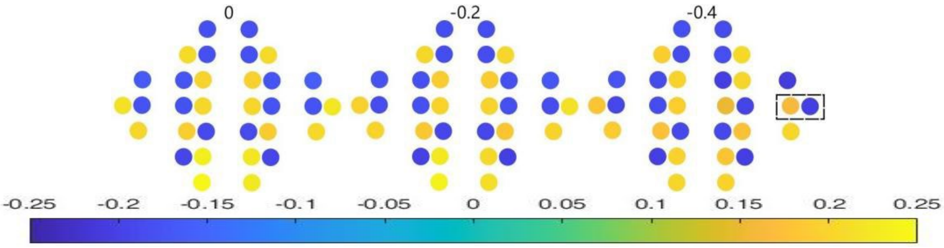


(a) (b)

Figure 1: (a) and (b) represent intact and defective silicon surfaces respectively. Si atoms that form dimers are shown in orange; The green atom in (b) is the atom that reparticipates in the construction of the new dimer after the defect; The remaining gray atoms are surface atoms that do not participate in the construction of dimers.

3. Data result processing

(1) Complete silicon surface: The charge map of the complete Si(100) surface is shown in Figure 2.



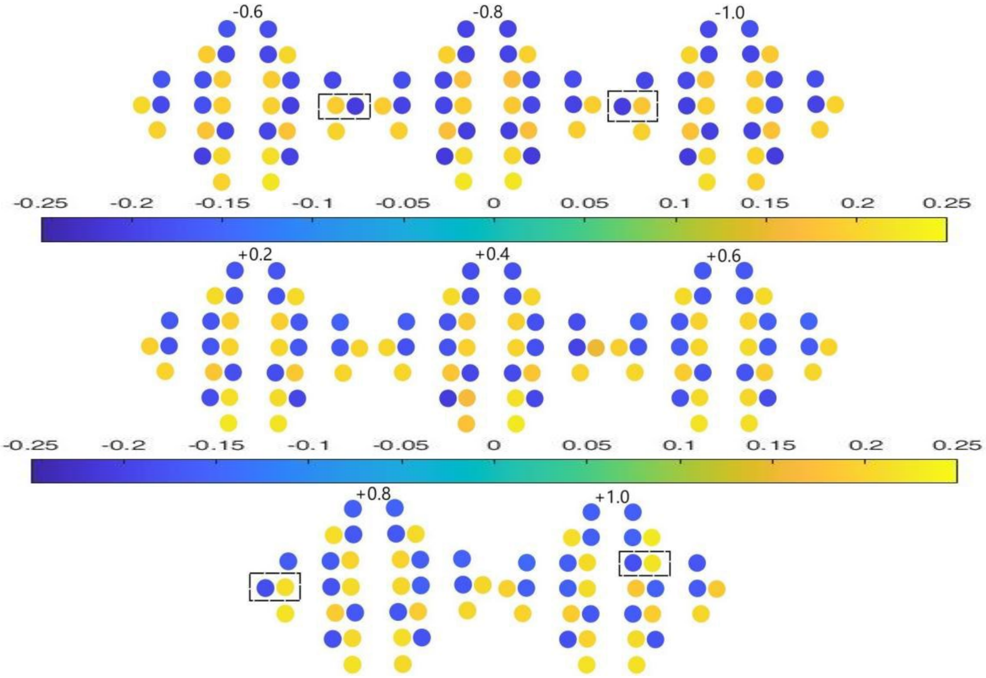


Figure 2: The population diagram is the complete surface charge distribution diagram of Si (100) under corresponding applied electric field intensity. Where the charge distribution changes significantly with no electric field applied are marked, and the intensity of the applied electric field is marked above the picture.

It is not difficult to find that, compared with the complete silicon surface charge distribution without an electric field, the charge distribution of part of the dimer obviously changes when the applied longitudinal electric field is -0.4v/m, -0.6v/m, -1.0v/m,+0.8v/m,+1.0v/m. Moreover, the twelve dimers formed on the silicon surface do not all satisfy the symmetrical distribution under the three applied longitudinal electric fields. Next, we analyze the main reasons for the apparent change in charge distribution.

First, when the applied electric field is -0.4v/m, its atomic structure is shown in Figure 3.

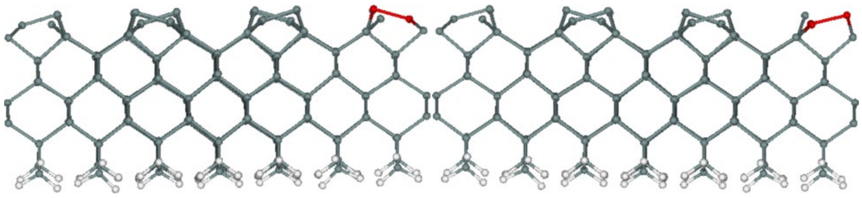
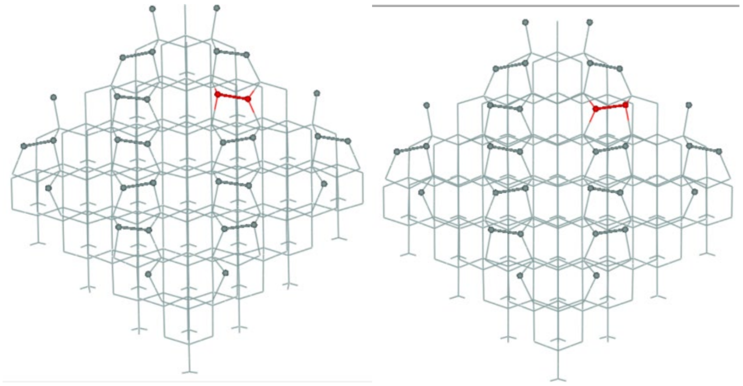

(a) (b)

Figure 3: (a) and (b) are the atomic structures when the applied electric field is not applied and when the applied electric field is -0.4v/m. The red atom is the one that changes under the applied electric field.

In Figure 3, two atoms are marked whose charge distribution is greatly altered by an applied electric field. The labeled atom (Si159) on the left has a charge of -0.1754e in the absence of an applied electric field and 0.1657e in the presence of an applied electric field of -0.4v/m. The labeled atom on the right (Si160) has a charge of 0.2236e in the absence of an applied electric field and -0.2047e in the presence of an applied electric field of -0.4v/m. The main reason why the charge distribution changes so much is that the atomic positions of Si159 and Si160 change under the intensity of the electric field. (See Table 1 for specific changes) Different from the above atomic changes under applied electric field, the above atoms have a symmetrical structure and all changes in the dimer composed of Si160 and Si159 and the symmetric dimers Si231 and Si232. When the applied electric field intensity is +1.0v/m, the change atoms occur inside the silicon surface atoms, Si191 and Si216, respectively. How this changes and the position of the changing atoms are shown in Figure 4.



(a) *(b)*

Figure 4:(a) and (b) are surface atomic structure diagrams when the applied electric field is +1.0v/m and no applied electric field, respectively. Atoms marked red are those that have changed positions; the remaining gray atoms are those whose surface has not changed.

In conclusion, when the longitudinal applied electric field intensity is -1.0v/m to +1.0v/m, atoms on the intact crystal silicon surface will change their positions when the electric field intensity changes. The x,y values of silicon atoms formed on the surface of the dimer do not change significantly after Cartesian coordinates are established in the center of the silicon crystal studied.The direction of the silicon atoms all changed to the Z value. After the change, the charge distribution of the dimer also changes greatly, thus breaking the original symmetrical structure of the charge distribution of the surface dimer. (Specific change data are shown in Table 1). Thus, it can be found that in the Si(100) flexion dimer, the upper dimer atom (Su) is generally electron rich, and the lower dimer atom (Sd) is generally electron deficient. Therefore, it can help us better understand and predict the chemical composition of silicon surface, and provide a theoretical basis for the treatment of adsorption systems later.

Tabel1: The picture shows the specific atomic information and the data of the charge quantity carried by the atom under the intensity of each applied electric field

Applied electric field intensity（v/m）	Serial number of Si	x value	Y value	Z value	The amount of charge that the Si atom has
0	159	28.9089	14.5097	59.8127	-0.17541369
	160	30.4719	12.8389	59.1332	0.22356806
	231	12.8366	30.4735	59.1495	0.21637819
	232	14.5045	28.9128	59.8157	-0.17707529
	191	28.0903	20.6781	59.8330	-0.17306830
	216	26.5195	22.3536	59.1721	0.19661012
-0.4	159	29.2030	14.2367	59.2252	0.16568562
	160	30.7949	12.5493	59.8239	-0.20468913
-0.6	159	29.2248	14.2382	59.1754	0.18899534
	160	30.8028	12.5492	59.8205	-0.20716604
-1.0	231	12.5475	30.8046	59.8344	-0.20716604
	232	14.2428	29.2173	59.1916	0.18194060
+0.8	231	12.5396	30.8037	59.8282	-0.18206717
	232	14.2298	29.2294	59.1620	0.21116530
+1.0	191	27.7596	20.9689	59.1727	0.21971309
	216	26.1809	22.6353	59.8717	-0.17870756

(1) Defective silicon surface Relative to the intact silicon surface, the molecular population of the defective silicon surface is shown in Figure 5 when the applied electric field ranges from -1.0v/m to +1.0v/m.

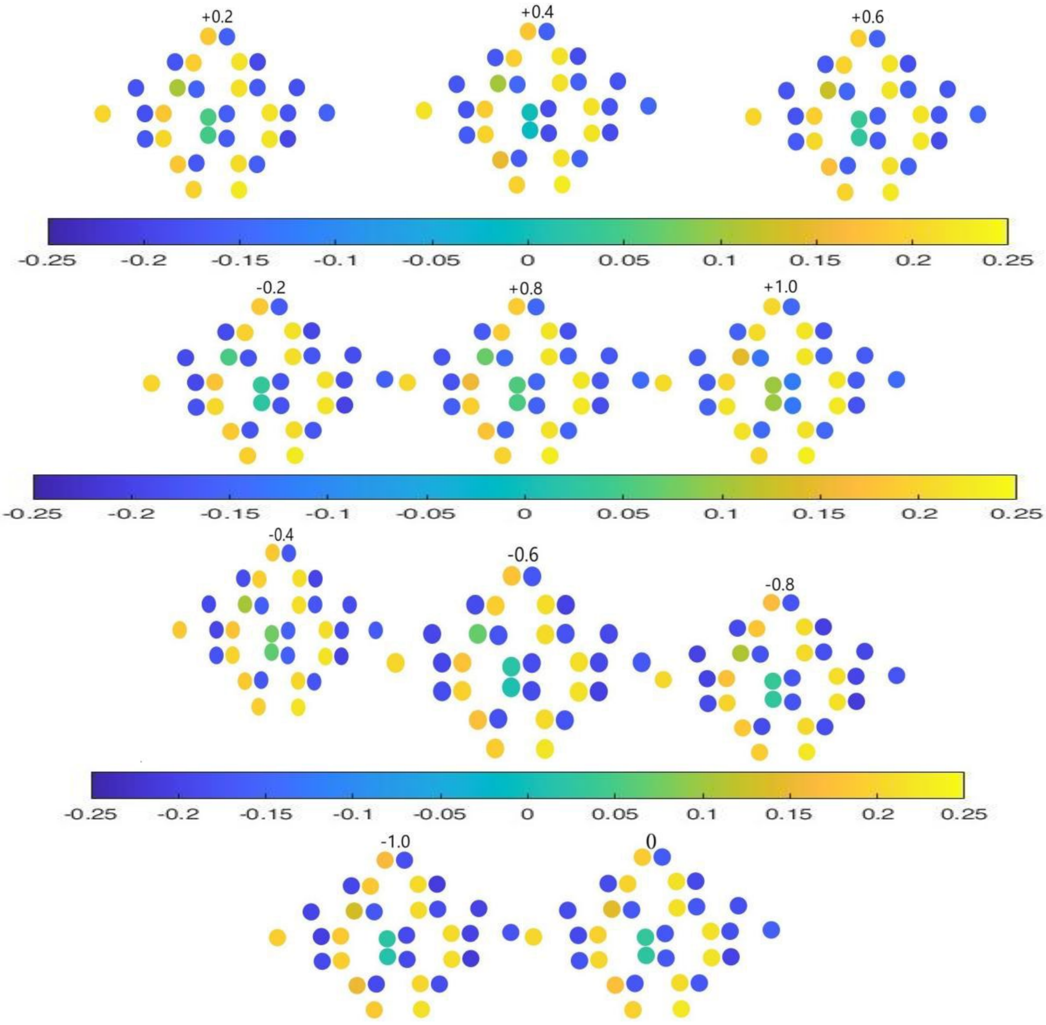


Figure 5:The population diagram is the surface charge distribution diagram of defect Si (100) under corresponding applied electric field intensity

Intact Si(100) has often been used in semiconductor substrate structures as opposed to defective Si(100) surfaces. Previously, there have been reports of defective silicon surfaces exhibiting four different reconstruction modes; Which includes c(21) [8–10] ,p(22) [11],c(42) [12,13] , and c(44) [14]. Chadi et al [15] confirmed that the (21) surface had the minimization energy, which was composed of a buck- led dimerpattern and some ionic bonds between these surface atoms. The main difference between them depends on the orientation of the bent dimer atoms. In the defect site of the flawed Si(100) surface, alterations manifest in the vicinity of the defect, which causes some dimer molecules to preferentially bind to the defective atom, while other atoms tend to the original surface site . Based on this, Chardy discovered that c(21) has the lowest energy on the surface. The restructured architecture comprises a pliable dimer and several ionic bonds among surface atoms. Moreover, the study on this defect pattern is more representative, which can provide some experimental data basis for the future surface adsorption problem.

For this reason, we mainly chose c(21) reconstruction mode for defect model reconstruction. However, it is not difficult to find that the charge distribution of some dimers on the previously treated defective silicon surface has some oscillating changes when applied to the electric field. For example, in the dimer composed of Si239and Si214, the charge transfer varies greatly. Therefore, we will analyze the charge change of the Si239 atom. Meanwhile, since Si239 and Si214 together form a dimer, the charge distribution of the two requires only the analysis of the change of charge distribution of one electron. Therefore, we have selected Si239 as the subject of our analysis and have included its charge distribution diagram in Figure 5.

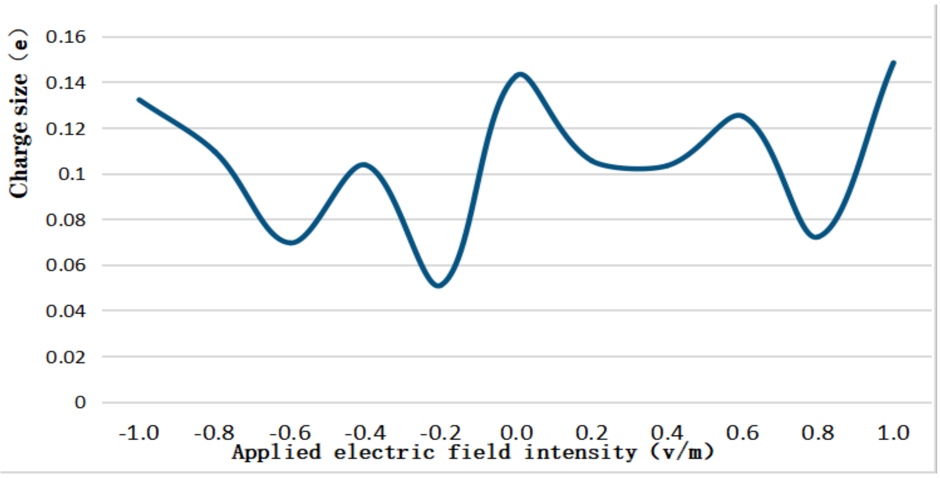


Figure 6: The figure shows the change of general charge distribution in the case of the c(21) defect. The charge distribution tends to oscillate with the constant change of applied electric field intensity

It is not difficult to see from Figure 6 and Figure 5. Whereas the charge distribution of the dimer in this defect mode does not change atomic properties (from electron- rich to electron-deficient). Under certain special applied electric field intensity as on the intact silicon surface, its charge distribution shows a tendency to oscillate. Therefore, on the c(21) defective silicon surface, we can predict the charge distribution of some atoms through the changes of different applied electric fields, so as to judge the strength of the Lewis acid base of the atom, which can provide some experimental basis and data basis in the subsequent selection of some adsorption sites.

4. Conclusion

Through an analysis of the surface atomic charge of both intact silicon surfaces and those with defective reconstruction, a significant alteration in the charged properties of select dimers on the intact silicon surface was observed under various applied longitudinal electric fields (-0.4v/m, -0.6v/m, -1.0v/m, +0.8v/m, and +1.0v/m). For the defective reconstructed silicon surface, under limited applied electric field intensity, the amount of charge carried by the surface atoms does not change much, but there is also a small range of charge transfers, and the charge transfer shows a trend of oscillating change.

The study of charge distribution on silicon surface affects the charge properties and charge intensity of the atom. It can affect the size of Lewisic acid and the base of the atoms involved, thus providing some theoretical and laboratory data basis for future research on surface adsorption. At the same time, studying the possible structure and charge distribution of the silicon surface can also increase our understanding of the Si surface from the electrical level.

References

[1] Zeng Hongjun. Analysis of Dangerous and harmful factors in polysilicon process [J]. Xin- jiang Chemical Industry, 2008, (4); 41-46.

[2] Duke Charles B. Semiconductor Surface Reconstruction: The Structural Chemistry of two-Dimensional Surface Compounds. [J]. Chemical reviews, 1996, 96(4).

[3] L. Zhang, Studying stability of atom packing for Ti nanoparticles on heating by molecular dynamics simulations, Adv. Eng. Mater. 21 (4) (2019) 1800531.

[4] Li Jing, Cui Yang, Zhao Dandan, Zhang Lin. C60 adsorption on Si (100) 21 reconstructed surface with single vacancy in sub-surface from DFTB algorithm [J]. Materials Science in Semiconductor Processing, 2022, 144.

[5] Seung.Chul Oh, Ki.Wan Kim, Ha.Jin Lee, Role of coverage and vacancy defect in adsorp- tion and desorption of benzene on Si (001)-2n surface, Bull. Kor. Chem. Soc. 317 (1) (2010) 162C167.

[6] J. A. Martin, D. E. Savage, W. Moritz, Structure, stability, and origin of (2n) phases on Si (100), Phys. Rev. Lett. 56 (18) (1986) 1936-1939.

[7] Hamers R. J., Tromp R. M., Demuth J. E., Scanning tunneling microscopy of Si(001)[J]. Physical Review B, 1986, 34(8).

[8] G. T. Wang, C. Mui, C. B. Musgrave, S. F. Bent, Competition and selectivity of organic reactions on semiconductor surfaces: reaction of unsaturated ketones on Si(100)- 21 and Ge(100)-21, J. Am. Chem. Soc. 124 (30) (2002) 8990C9004.
[9] R. Konecny, D. Doren, Theoretical prediction of a facile diels-alder reaction on the Si(100)- 21 surface, J. Am. Chem. Soc. - J AM CHEM SOC 119 (1997).
[10] P. Minary, M. Tuckerman, Reaction pathway of the [4 + 2] dielsalder adduct formation on Si (100)-21, J. Am. Chem. Soc. 126 (2004), 13920.
[11] K. Hata, S. Yoshida, H. Shigekawa, p(22) phase of buckled dimers of Si(100) observed on n-type substrates below 40 K by scanning tunneling microscopy, Phys. Rev. Lett. 89 (28) (2002).
[12] M. Mantega, I. Rungger, B. Naydenov, J. J. Boland, S. Sanvito, Spectroscopic characterization of a single dangling bond on a bare Si(100)-c(42) surface for n and p-type doping, Phys. Rev. B 86 (3) (2012), 035318.
[13] J. E. Northrup, Dimer-plus-chain structure for the Si(100)-c(42) surface, Phys. Rev. Lett. 54 (8) (1985), 815-818.
[14] J. Y. Lee, M. H. Kang, Structure and bonding nature of C60-Si(100)c(44): density functional theory calculations, Phys. Rev. B 75 (12) (2007) 125305.
[15] D. J. Chadi, Atomic and electronic structures of reconstructed Si (100) surfaces, Phys. Rev. Lett. 43 (1) (1979) 43-47.