Posudek práce

předložené na Matematicko-fyzikální fakultě
Univerzity Karlovy

❑ posudek vedoucího ☒ posudek oponenta
❑ bakalářské práce ☒ diplomové práce

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Název práce:	Modification of silicon surfaces for selective adsorption
Studijní program a obor:	Physics, Physics of surfaces and Ionized Media
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Odborná úroveň práce:
❑ vynikající ☒ velmi dobrá ❑ průměrná ❑ podprůměrná ❑ nevyhovující

Věcné chyby:
☒ téměř žádné ❑ vzhledem k rozsahu přiměřený počet ❑ méně podstatné četné ❑ závažné

Výsledky:
☒ originální ❑ původní i převzaté ❑ netriviální kompilace ❑ citované z literatury ❑ opsané

Rozsah práce:
❑ veliký ☒ standardní ❑ dostatečný ❑ nedostatečný

Grafická, jazyková a formální úroveň:
❑ vynikající ☒ velmi dobrá ❑ průměrná ❑ podprůměrná ❑ nevyhovující

Tiskové chyby:
❑ téměř žádné ❑ vzhledem k rozsahu a tématu přiměřený počet ☒ četné

Celková úroveň práce:
❑ vynikající ☒ velmi dobrá ❑ průměrná ❑ podprůměrná ❑ nevyhovující

Slovní vyjádření, komentáře a připomínky oponenta:

The reviewed work (Modification of silicon surfaces for selective adsorption) presents the study of the interaction of organic molecules with modified silicon surfaces. Author uses the scanning tunneling microscope (STM) to probe the behavior of different phthalocyanine molecules on the Si(111) surface modified by tin and indium. The focus of the study is given to "fuzzy" adsorption configurations of H_2Pc and F_8CuPc molecules, which are foreseen as potential two-state molecular switches.

The theoretical part of the work is well-composed: it suitably complements the experimental part.

The experimental part of the work includes STM images, scanning tunneling spectra and time series of the fluctuating tunneling current measured above "fuzzy" molecules. These experimental data are analyzed in order to determine the adsorption model and to clarify the nature of the fuzzy behavior. As a result of the analysis, the "fuzzy" molecules are identified as spontaneous thermally activated two-state molecular switches. Two possible switching models are suggested and discussed.

The results of the thesis are original and well-presented. The extent of the work is sufficient. The motivation for the study is explained only vaguely. A more detailed explanation of the motivation would be appreciated, especially since the author wrote that only the non-spontaneous molecular switches are interesting for applications in molecular electronics.

The author should pay more attention to the typographical correction of the thesis. The text contains a lot of typos (missing gaps, misspelling, grammatical errors etc.). Although it does not change the scientific value of the thesis, it significantly lowers the impression from reading.

Other minor and major remarks are listed in the text below.

Overall, I recommend the thesis as a master thesis after the successful defence.

Minor remarks:

Page 25, fig. 4.2: What does “[htbp]” in the title of the figure mean? What does “wrt” in the description of the y axis mean? These abbreviations are not clearly explained in the text.

Page 25, section 4.1.1: You state that “Positive charge (in figure 4.2) is denoted with red colour and negative charge with blue or green colour. ”. What do you mean by a “positive charge”?

Page 30, fig. 4.5: The scanning direction should be marked. What does the controlled approach of the tip mean? What are the scanning conditions in all three consecutive images? (The molecule marked by the blue arrow on the first image and the first half of the same molecule on the second image looks differently.)

Page 32, fig. 5.2: The orientation of the evaporators “a2” and the shape of the corresponding molecular beam are misleading.

Page 37, fig. 6.1: Rows in the STM images are not aligned. Terrace planes are not leveled.

Page 50 – page 54: All normalized dI/dV spectra, except the spectrum in fig. 6.13, have the y axis called “(dI/dV)(I/V)” .

Page 69 – page 74: Inconsistent formatting of references in the bibliography. Frequent typographical errors.

Případné otázky při obhajobě a náměty do diskuze:

In the section 3.1 (page 16), you describe the term "surface passivation" as "the tool for saturating the surface dangling bonds and decrease the reactivity of the surface". In the next section, you use tin as an example of the passivation agent. Does deposition of tin atoms on the silicon surface satisfy this definition, as tin and silicon atoms have the same number of valence electrons? Does deposition of the tin decrease the reactivity of the surface?

Figure 3.4 (page 18, reprinted from ref. [25]) displays the STM image of the Sn/Si(111) surface and its basic types of defects – Si substitutions, vacancies and Sb substitutions. The figure shows that there can be a relatively big portion of Sb substitutions compared to the vacancies and Si substitutions. In the figure 3.9 (page 22, your STM image), you mark only vacancies and Si-substitution defects. Can you estimate the ratio between the surface coverage by the three types of defects on your Sn/Si(111) and In/Si(111) surfaces? Did you observe multiple types of adsorption configurations on different types of defects? How did you confirm the type of defects under the adsorbed molecules?

On the page 36, you wrote that only the two-state molecular switches that are reversible and non-spontaneous are interesting for applications in molecular electronics. Did you observe any non-spontaneous (i.e. controlled) switching in your studied systems? If not, what is your primary motivation in studying such spontaneous molecular switches?

Page 41: You wrote: "H_2Pc molecules at low coverage adsorb not only on Si-substitution double defects (fuzzy appearance) but also on Si single defects and multiple defects (see Fig. 6.5).". How did you distinguish the type of defects underneath the adsorbed molecules from the Fig. 6.5.?

Page 49 and 54: During your measurements of dI/dV spectra, you measured the reference spectra of the clean Sn/Si(111) surface. To prove the correctness of your dI/dV spectra, you compared the positions of the peaks in your spectra with the already published spectra from fig. 3.5 and ref [65]. However, two reference spectra in figure 6.16 have different positions of the peaks (it seems that the small gap around the Fermi level is not the only difference between the two displayed spectra). Can you explain this discrepancy?

Page 62: You wrote: "Even though we had measured the I-V curve (above fuzzy molecules), careful separation of both states and subsequent differentiation was not possible from our measurements." Can you please show the example of the I-V curve measured above a fuzzy molecule? Can you discuss the reasons why the separation of the two states is not possible, even though you measure above the thermally-activated two-state molecular switch (the molecular switch that permits you to measure the two-level fluctuations of the tunneling current at different voltages)? … "Previous measurements of I-V [65] showed splitting of the curve for the low and the high state …". Can you show the I-V curve with the splitting?

Page 63: In the discussion you suggested that the molecular switch can be realized by the H_2Pc or CuPc molecule translating along the axis a_{dd} with the center of the molecule closer to one or to the other Si atom in the two states. You wrote that "the resulting change of the electronic structure between the two mirror-symmetric adsorption positions can be significant and can result in a large change in the tunneling current.". In this case, if you assume that the two states have significantly

different electronic structures, how do you explain that the fractional population of both states is equal to 0.5?

Page 64: In your explanation of the influence of the tip on the fuzzy behavior of the molecules with a non-zero permanent dipole you assumed that the radius of tip is more than 50 nm and the electric field close to the tip can be therefore considered homogeneous. Can you please provide a schematic drawing that clarifies how such a locally homogeneous electric field alters the double-well potential in the way that it results in the change of the switching frequency?

Práci
☒ doporučuji
❑ nedoporučuji
uznat jako diplomovou.

Navrhuji hodnocení stupněm:
❑ výborně ❑ velmi dobře ❑ dobře ❑ neprospěl/a

Místo, datum a podpis oponenta: