Posudek práce

předložené na Matematicko-fyzikální fakultě
Univerzity Karlovy

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

Autor/ka: Benjamín Andreides
Název práce: Modelling of precursors for electron-beam induced deposition
Studijní program a obor: Fyzika, Biofyzika a chemická fyzika
Rok odevzdání: 2022

Jméno a tituly vedoucího/oponenta: Dr. Juraj Fedor, PhD
Pracoviště: Ústav fyzikální chemie J. Heyrovského AVČR
Kontaktní e-mail: juraj.fedor@jh-inst.cas.cz

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 vedoucího/oponenta:

The thesis of Bc. B. Andreides deals with the computational treatment of fragmentation of iron pentacarbonyl following its dissociative ionization. The motivation for this work is two-fold. The first is the general need to understand the precursor decomposition in the focused-beam nanofabrication. The second are the specific experimental data about the fragmentation of $Fe(CO)_5$ which has been recently measured in our laboratory and the explanation of which requires a computational approach such as the one presented in the thesis.

The thesis is well structured. The relatively brief introduction (chapter 1) describes the FEBID technique and molecular properties of $Fe(CO)_5$. This is followed by much more extensive introduction into the computational techniques which were used for the current simulations. The student used the software package MBN Explorer, in chapter 2 he describes in detail the implementation of the potentials and of various aspects of molecular dynamics simulations in this package. Chapter 3 is the most important one: here the student describes the results which he obtained and compares them to the available experimental data (where applicable). The thesis is wrapped up by a short conclusion section.

The results are undoubtedly interesting. The first simulated system was isolated iron pentacarbonyl cation where the main quantity – appearance energies of fragments – are in an excellent agreement with the experiment. The second simulated system was iron pentacarbonyl cation deposited on a large argon cluster. Here, in agreement with the experiment, a quenching of the fragmentation is observed. The last simulated system concerned landing of a metal nanoparticle embedded in an argon cluster on a substrate. The goal was to find out whether argon prevents deposition of the particle. The simulations showed that it does so only under very specific circumstances which would be hard to achieve experimentally.

Strengths of the thesis:

- This is a previously unexplored topic. The student had to apply the software in the new direction which required considerable effort and creativity.
- The simulations bring certain information which is not accessible experimentally, e.g., position of the dopant in the argon cluster or the behaviour of the landing metal nanoparticle. This immensely helps in the interpretation of the experiments.
- The amount of original results is very high. The thesis is a base of a journal publication which is currently being finalized.

Weaknesses of the thesis.

- Many effects which are observed in the simulations could have been explained better, in quite a few places I am missing a physical insight into the observed phenomena.
- The balance between the individual chapters is not very good, the description of MD simulations is much more extensive than the description of results. This is connected with the previous point.
- The language style which the student uses (e.g., specific terminology) in many cases does not correspond to established terms.
- The quality of the figures is low. Also, throughout the whole thesis, the labels in the figures use neutral notation of the fragments, while in reality these are all cations.

In conclusion, I suggest that the commitee accepts this work as a diploma thesis. As a compromise between the excellent results and the relatively weak adaptation into the text, I suggest to evaluate it with the second best grade, very good.

Případné otázky při obhajobě a náměty do diskuze:

The basic assumption in the model is that upon ionization, the iron pentacarbonyl cation is created in its ground electronic state and the excess energy is given into the vibrational motion. How realistic is this assumption?

For the isolated molecule, the main experimental benchmark are the appearance energies of individual fragments. What type of experiment would be necessary to verify simulation fully, i. e., to record a fragmentation pattern as a function of the cation excess energy?

One of the main results is quenching of the iron pentacarbonyl fragmentaion by the environment. What are the implications of this effect for FEBID and its simulations?

Práci
☒ doporučuji
❑ nedoporučuji
uznat jako diplomovou.

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

Místo, datum a podpis vedoucího/oponenta:
Praha, 10. 8. 2022