Simple atomistic modeling of adsorptions on various surfaces

The project description should be in English and contain the following points:

1. Introduction:

Formulation of the scientific problem the project is related to, a list of scientific research conducted in this area, a story about applied problems.

Synthesis of new elements of the periodic table of elements is the ongoing experimental work at FLNR JINR (1). Technically, the experimental setup contains detector where a synthetized species or it compounds adsorbs. From that, simply saying, experimentalists deduce adsorption enthalpies.

Here, the computational molecular physics can render assistance to experimentalists. Adsorptions of superheavy elements (SHEs), their lighter homologues and their various compounds on detector surfaces (like gold, quartz, selenium and others) can be modelled at the atomic level.

The candidate will utilize open-source computational physics tools for fast and automated modeling of adsorptions. The methodology - atomistic simulations - is based on interatomic interactions' models, each provided with a given set of interactive potentials.

The computational workhorse for the project is ASE - Atomic Simulation Environment (2) with connected codes to simulate adsorption processes of modeled adsorbates and surfaces.

Student is supposed to install and run ASE Python codes on his own personal computer (notebook).

References

(1) Synthesis and Properties of Superheavy Elements, Structure of Nuclei at the Limits of Nucleon Stability, Project code 03-5-1130-1-2024/2028, in TOPICAL PLAN FOR JINR RESEARCH AND INTERNATIONAL COOPERATION 2025, Dubna, https://www.jinr.ru/wp-content/uploads/JINR_Docs/JINR_Topical_Plan_2025%20(eng).pdf

(2) https://wiki.fysik.dtu.dk/ase/ The Atomic Simulation Environment (ASE) is a set of tools and Python modules for setting up, manipulating, running, visualizing and analyzing atomistic simulations. The code is freely available under the GNU LGPL license.

2. Main part:

Here you need to list what the internship participant will learn and what he will learn.

Participant shall perform the atomistic modeling via simple Python codes in ASE, using only computationally fast models of interatomic potentials.

He will learn how to use ASE. Likewise, he shall do Python programming in the ASE framework.

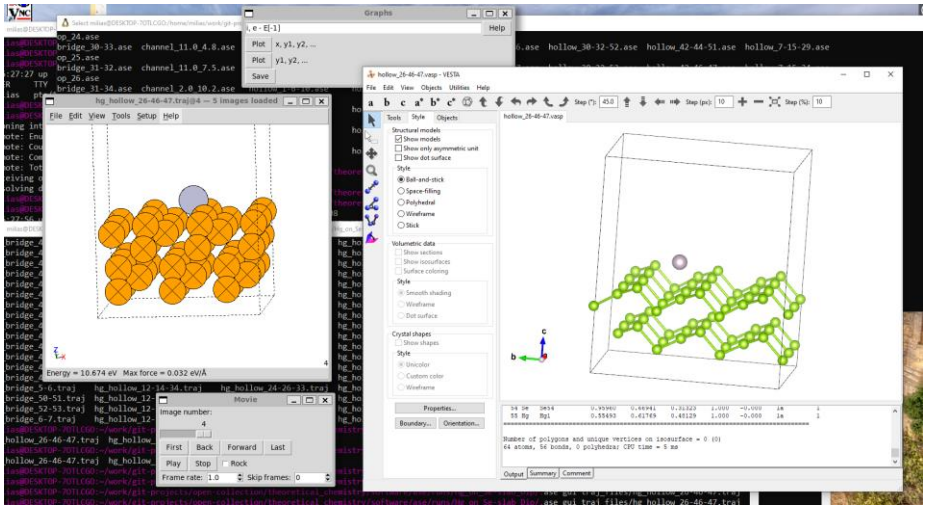
3. Description of the work on the project:

3.1. Installation (photo and diagram);

Student shall install the WSL2 Linux emulator if he has MS Windows operating system on his personal computer/notebook.

In the Linux environment he shall install ASE program, via pip command, and run self-tests.

Afterwards, he shall use run the sample code, https://github.com/miroi/open-collection/tree/master/theoretical_chemistry/software/ase/runs/Hg_on_Se-slab_Dip , which models all mercury atom positions on the periodic Selenium surface:



3.2. Measurement procedure (what the student needs to do);

Student shall proceed – **under the guidance of project managers** – with modifying the template code, https://github.com/miroi/open-collection/tree/master/theoretical_chemistry/software/ase/runs/Hg_on_Se-slab_Dip to incorporate other types and sizes of surfaces, for different adsorbates and for different interatomic models.

3.3. Form of presentation of results.

Results are in both the form of functional Python-ASE codes and in the form of codes outputs - graphical, alphanumerical. Graphical outputs are pictures of adsorbates on surfaces, alphanumerical outputs are tables containing adsorption energies of species on modelled surface, under specific atomistic simulation parameters.

4. Requirements for the level of student training.

We expect senior student (Master of PhD.), with the background of physics (molecular). Experience with Python programming is mandatory.

5. Recommended literature in English.

As to the literature, this the web page related to the computational apparatus: https://wiki.fysik.dtu.dk/ase/

Then there are the experimental papers related to synthesis of new elements and their adsorptions on surfaces:

https://link.springer.com/article/10.1007/s10967-016-5018-8

https://www.tandfonline.com/doi/full/10.1080/00268976.2023.2272685#d1e686

6. Number of project participants:

How many students at the same time, individually or in a team, can work on the project.

Number of students: **2**

7. Project manager(s) from JINR:

Full name, photo (optional), position, academic title, laboratory, department, scientific interests, available scientific results, link to individual web page).

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Attention! The project description with photos and drawings should be no more than 3-4 pages.

When preparing the project, remember that it:

- *should reflect the topic of research conducted at JINR;*
- *should be feasible within 3 weeks;*
- *should not repeat the tasks of physics practical training for students at universities.*

Your participation in working with students during the practical training is paid.