Python driven simple atomistic modeling of mercury adsorption on gold surface

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1 Introduction

The synthesis of new elements of the periodic table is ongoing experimental work at the Flerov Laboratory of Nuclear Reactions at the Joint Institute of Nuclear Research [1]. Technically, the experimental setup contains detectors where a synthesized species or their compounds adsorb. From that, simply said, experimentalists are able to estimate adsorption enthalpies.

Here, computational molecular physics can provide assistance to experimentalists. Adsorption of superheavy elements (SHEs), their lighter homologues, and their various compounds on detector surfaces (such as gold, quartz, selenium, and others) can be theoretically studied at an atomic level using methods of computational molecular and materials physics.

The candidate will utilize available open-source computational physics tools for fast and automated modeling of adsorptions. Its methodology—atomistic simulations—is based on interatomic interaction models, each accompanied by a set of interactive potentials.

The computational workhorse for the project is the Atomic Simulation Environment (ASE) [2, 3] with connected codes to simulate the adsorption processes of selected adsorbates and surfaces.

Students are supposed to install and run ASE Python codes on their own personal computers (notebooks).

1.1 References

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2 Main part

Program participants shall perform simple and computationally fast atomistic simulations using Python programs in ASE. They shall employ available machine-learned interatomic potentials [4, 5]. We stress that machine learning, as part of the artificial intelligence, is the subject of development in the Russian federation [6, 7].

Students will also learn how to use the above mentioned ASE, and, eventually, do simple Python programming in the ASE framework.

Likewise, experimentalists in the sector of Dr. Nikolay Victorovich Aksenov from the Flerov Laboratory of Nuclear Reactions at JINR can provide consultations concerning the synthesis of superheavy elements and their adsorption on detector surfaces, according to their convenience.

3 Description of the work on the project

3.1 Installation (photo and diagram)

Students shall install the WSL2 Linux emulator onto their personal computers if they have the Microsoft Windows operating system. Next, in the Linux environment (either native or WSL2) of their personal computers, they shall install the ASE program and related dependencies.

Afterwards, they shall run the sample codes[8], which model mercury atom and mercury cluster adsorption on the periodic gold (111) surface - see Figure 1 and Figure 2 .

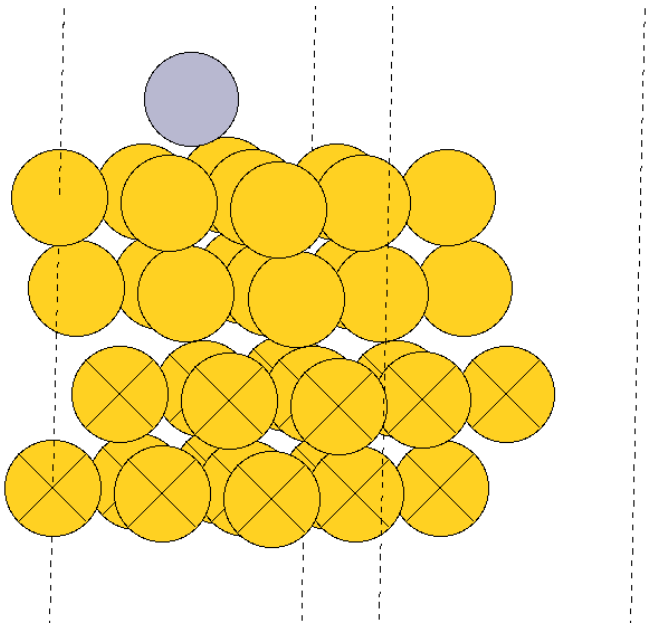

Figure 1: Mercury atom adsorbed on the gold surface. Obtained with ASE.

3.2 Measurement procedure (what the student needs to do)

Students shall proceed – under the guidance of project leaders– with modifying the template codes[8] to incorporate other types and sizes of surfaces, for differently sized 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 outputs from those codes – both graphical and alphanumerical.

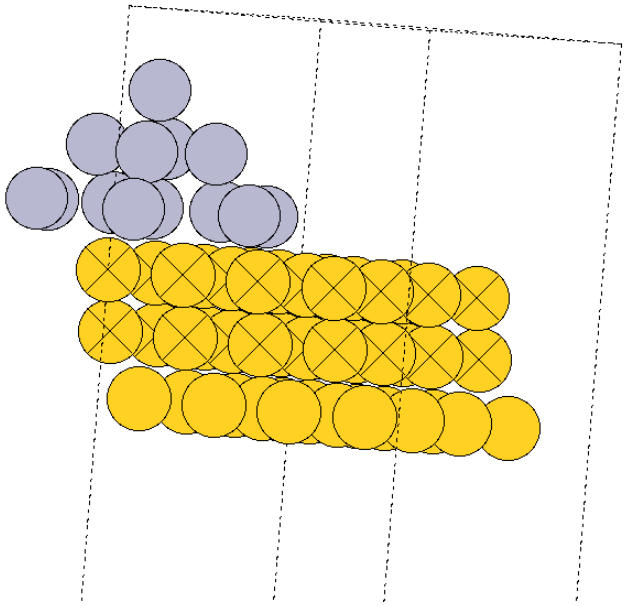

Figure 2: Cluster of mercury atoms adsorbed on the gold surface. Obtained with ASE.

Graphical outputs are pictures of adsorbates on surfaces.

Alphanumerical outputs are tables containing the adsorption energies of species (mercury atom and mercury cluster) on the gold surface, under specific atomistic simulation parameters.

4 Requirements for the level of student training

We expect senior students (Master or PhD), with the background of physics (molecular) or chemistry. Experience with Python programming is welcome.

5 Recommended literature in English

We recommend the paper on the theoretical adsorption study of elements, including Hg, on several surfaces, including gold [9].

Then the literature about the employed computational apparatus [2, 3, 4] is all mentioned in Section 1.1.

6 Number of project participants

We suggest two students, but there can also be three students. All shall be working in one team.

7 Project manager(s) from JINR

Figure 3: Miroslav Iliaš, Leading research scientist, PhD., BLTP JINR (https://pin.jinr.ru/p?jid=19119), computational molecular and materials physics, ORCID: https://orcid.org/0000-0002-8038-6489

Figure 4: Dipayan Sen, Senior research scientist, PhD., BLTP JINR (https://pin.jinr.ru/p?jid=20306), computational molecular and materials physics, ORCID: https://orcid.org/0000-0002-9864-0692