Interatomic Potentials Based Computations of Atomic Adsorption Energies on Gold Surfaces

Miroslav Iliaš[1] **and Dipayan Sen**[2]

[1]BLTP JINR, 6 Joliot-Curie Street, 141980 Dubna, Moscow Region, Russia , milias@theor.jinr.ru
[2]BLTP JINR, 6 Joliot-Curie Street, 141980 Dubna, Moscow Region, Russia , dsen@theor.jinr.ru

February 17, 2026

1 Abstract/brief description

The gold surface is used as a detector cover in the preparation of superheavy elements in one-atom-at-a-time experiments, a complicated process also conducted here in the Flerov Laboratory of Nuclear Reactions at JINR in Dubna.

There, synthesized atoms and their possibly formed molecules adsorb onto the gold surface, and experimentalists estimate their adsorption enthalpy.

To shed more light on the process at an atomic level, computationally feasible, simple atomistic modeling with the Atomic Simulation Environment tool (ASE, `https://ase-lib.org/`) is utilized to predict adsorption energies and even adsorption enthalpies of atoms. This open-source methodology is based on interatomic potentials (IP), spanning from the simplest (like Lennard-Jones) to sophisticated machine-learned ones (ML-IP).

This project, lasting for 6 weeks, is co-supervised by Dr. Dipayan Sen from BLTP JINR.

2 Tasks

- Setting up Linux environment on the participant's personal computer
- Installing and testing ASE on the participant's personal computer
- Download and run the ASE demonstration programs from the open repository `https://github.com/miroi/open-collection/tree/master/theoretical_chemistry/projects/adsorptions_with_ase`
- With the help of the supervisor, modify the provided programs

- With the adapted programs, conduct adsorption calculations
- collect and process the computed results; write the report in Overleaf

3 Preliminary schedule by topics/tasks

- Week 1: Install and test ASE on your personal computer
- Week 2: With the supervisor's help, modify the programs from the repository `https://github.com/miroi/open-collection/tree/master/theoretical_chemistry/projects/adsorptions_with_ase`
- Week 3: Modify and run the program for the adsorption of various atoms
- Week 4: Collect results, such as computed energies, final geometries, pictures of converged structures, etc.
- Week 5: Start writing the report in Overleaf
- Week 6: Finalize the report with the supervisor's help

4 Required skills

- Install and test ASE on your personal computer
- Download and run the demonstration software from the open repository
- With the help of the supervisor, modify the provided software
- With the modified software, run more calculations

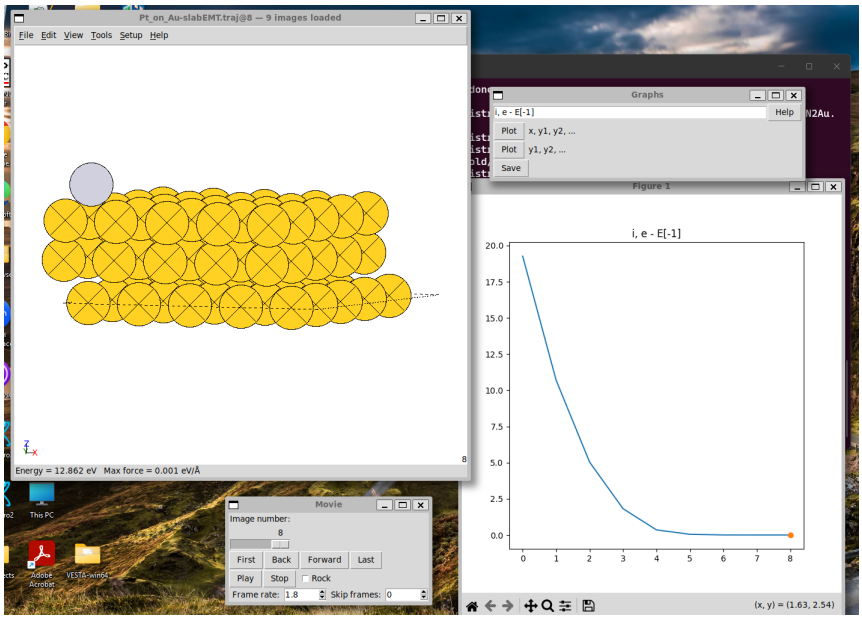
5 Acquired skills and experience

- Mastering Linux administration on one's personal computer
- Mastering the installation and testing of ASE and related packages
- Improving programming skills in Python
- Learning the basics of atomistic modeling in ASE
- Learning to set up adsorption simulations in ASE for the calculation of adsorption energies
- Mastering Overleaf for report writing

6 Recommended literature

- Atomic Simulation Environment webpage, https://ase-lib.org, with tutorials and references therein,
- The Web Python Tutorial, https://docs.python.org/3/tutorial/index.html
- Alfred Clark : The theory of adsorption and catalysis (Physical chemistry, a series of monographs) 0th Edition, Academic Press, 1970, 418 pages, ISBN 978-0121754501
- Yu. K. Tovbin : The Molecular Theory of Adsorption in Porous Solids, CRC Press, 2017, 780 pages, ISBN 9781351649711

7 Project photo



8 Full project description

Gold surfaces exhibit unique adsorption characteristics, often acting as a relatively inert and noble metal substrate for physical adsorption. On the other hand, it shows high reactivity and strong chemisorption properties when present in the form of nanoparticles or when interacting with specific functional groups like thiols. Key gold surface characteristics include, for example, a strong affinity for sulphur, high surface mobility of atoms, and dependency on surface structure (e.g., crystal face, steps, kinks).

As for the crystal structure type, Au(111) represents the closest-packed, low-energy surface plane of face-centered cubic (FCC) gold, exhibiting 3-fold symmetry with a hexagonal atomic arrangement. As it is the most thermodynamically stable and smooth surface, it is a common subject in surface science studies. However, depending on how the gold crystal is cut or grows, different atomic arrangements—called facets—emerge at the surface. For example, Au(100), a square lattice of atomic surfaces, is less stable than the (111) form and often reconstructs into a quasi-hexagonal top layer that sits mismatched over the square bulk. Alternatively, Au(110) is an open, "ridged" structure with rows of atoms that typically undergo a missing-row reconstruction, where every second row of atoms is absent, creating a (1x2) periodicity.

In the Flerov Laboratory of Nuclear Reactions (FLNR) at JINR - the gold surface is employed as the primary substrate in gas-phase thermochromatography detectors to study the chemical properties of superheavy elements (SHE).

Various interatomic potential (IP) methods, ranging from classical empirical force fields to advanced machine-learning models, are of interest here for theoretical studies of adsorption on gold surfaces. This is because they are feasible and fast on ordinary personal computers, in contrast to hardware-demanding quantum-mechanical methods, such as Density Functional Theory (DFT), for which we need powerful supercomputers.

In this project, simple atomistic interatomic potential based computations are employed to model the adsorption of selected atoms on the gold surface. The principal theoretical tool for this task is the popular, open-source Python library "Atomic Simulation Environment" (ASE, `https://ase-lib.org/`) along with all connected modules. With ASE, one can model not only the most stable crystallographic form of the gold surface, fcc(111), but also other facets.

Project participants work with ASE on their personal computers. For that, they download the free template Python programs from the supervisor's open repository (`https://github.com/miroi/open-collection/tree/master/theoretical_chemistry/projects/adsorptions_with_ase`) and modify them accordingly for different add-atoms, types of gold surfaces, and available IP methods in the vast ASE ecosystem.