Python-Based Fast Screening of Molecular Adsorption Sites on Gold Surfaces

Dipayan Sen, Miroslav Iliaš

February 2026

1 Abstract/brief description

Gold surfaces serve as the standard detector coating for one-atom-at-a-time superheavy element synthesis as typical experimental process conducted at the Flerov Laboratory of Nuclear Reactions (JINR, Dubna). Here, synthesized atoms and their potential molecular compounds adsorb onto the gold surface, enabling experimental determination of adsorption enthalpies.

To model this process at a fundamental level, under wave 14, INTEREST, we will employ the Atomic Simulation Environment (ASE, https://ase-lib.org/) for rapid screening of small molecules on detector surfaces and predict stable configurations and adsorption energies. Our open-source workflow leverages interatomic potentials ranging from simple Lennard-Jones to sophisticated machine-learned variants to bridge empirical screening and first-principles accuracy.

This project is co-supervised by Dr. Miroslav Iliaš from BLTP JINR.

2 Tasks

- Set up a Linux environment on the participant's personal computer
- Install and test the Atomic Simulation Environment (ASE)
- Download and run ASE demonstration programs from the provided open repository (`https://github.com/miroi/open-collection/tree/master/theoretical_chemistry/projects/adsorptions_with_ase`)
- Modify the sample programs under supervisor guidance
- Perform adsorption calculations using the adapted programs
- Collect and process the computational results; compile the final report

3 Preliminary schedule by topics/tasks

- Week 1: Install and test ASE on the participant's computer
- Week 2: With supervisor guidance, modify programs from the provided open repository (`https://github.com/miroi/open-collection/tree/master/theoretical_chemistry/projects/adsorptions_with_ase`)
- Week 3: Study surface adsorption using different molecules and potentials
- Week 4: Study surface adsorption using different molecules and potentials
- Week 5: Study surface adsorption using different molecules and potentials
- Week 6: Finalize the report with supervisor feedback

4 Required skills

- Basic Linux command proficiency
- Familiarity with GitHub and version control systems
- Basic Python knowledge

5 Acquired skills and experience

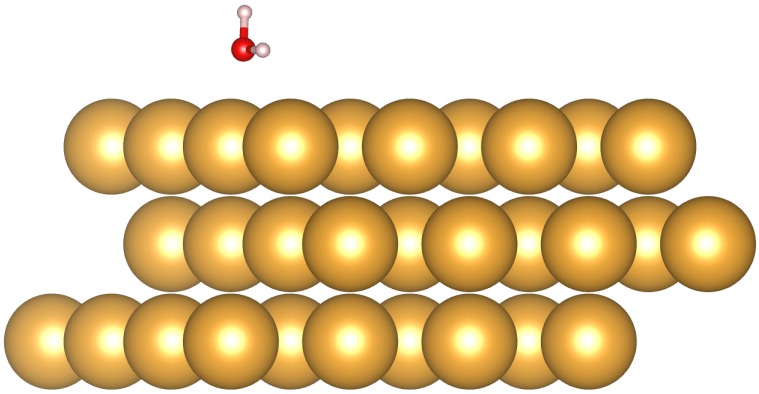
- Gain proficiency with Linux administration on the the participant's personal computer
- Mastering installation and testing of ASE and related packages
- Improving Python programming skills
- Acquire understanding of atomistic modeling using ASE
- Learn to configure adsorption simulations and calculate adsorption energies
- Gain proficiency with LaTeX 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. As a relatively inert and noble metal substrate, gold typically facilitates physical adsorption. However, it demonstrates high reactivity and strong chemisorption properties when in the form of nanoparticles or when interacting with specific functional groups such as thiols. Key characteristics of gold surfaces include a strong affinity for sulfur, high surface mobility of atoms, and structural dependency—for instance, on crystal face, steps, and kinks.

The Au(111) surface is the closest-packed, low-energy plane of face-centered cubic (FCC) gold. It exhibits 3-fold symmetry and a hexagonal atomic arrangement, making it the thermodynamically most stable and hence a commonly modeled system in surface science. However, different atomic arrangements, known as facets, may emerge depending on how the gold crystal is cut or grown. Au(100), for instance, presents a square atomic lattice and is less stable than the Au(111); it often reconstructs itself into a quasi-hexagonal top layer mismatched over the square bulk. Au(110), in contrast, features an open, "ridged"

structure, and it typically undergoes a missing-row reconstruction, resulting in a (1x2) periodicity.

In the Flerov Laboratory of Nuclear Reactions (FLNR) at JINR, gold surfaces serve as the primary substrate in gas-phase thermochromatography detectors for studying the chemical properties of superheavy elements (SHE). Hence, this project focuses primarily on modeling simple molecular adsorption on gold.

In the current project, participants will work in a local Linux environment on their personal computers. The principal computational tool for this task is the open-source Python library Atomic Simulation Environment (ASE, `https://ase-lib.org/`) and its associated modules. ASE provides a unified framework for modeling adsorption across diverse surfaces, molecular adsorbates, and interatomic potentials.

In contrast to demanding quantum-mechanical methods such as Density Functional Theory (DFT), which require powerful supercomputers, this approach will focus on fast screening of adsorption using various interatomic potential (IP) methods. These may range from classical empirical force fields to advanced machine-learning models. Such approaches are advantageous because: 1) they can be executed on a personal computer, and 2) the results can serve as a preliminary step for more intensive and accurate quantum chemistry computations.

As part of the project, the participants will download 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 adsorbates, gold surface types, and interatomic potential methods available within the ASE ecosystem.