



# THE UNIVERSITY *of* EDINBURGH

## Job Description

**Internship Title:** NERC Research Experience Placement - Employ.ed on Campus - Bringing Atomic-level insights to Caesium Decontamination by Clay Minerals

<b>Department / School</b>	School of Chemistry, University of Edinburgh
<b>Reports To</b>	Dr Valentina Erastova, School of Chemistry, University of Edinburgh - valentina.erastova@ed.ac.uk

### Job Purpose

The student will investigate the adsorption of Cs-137 onto montmorillonite and vermiculite clays at atomic-level resolution. They will use molecular dynamics (MD) simulations, a theoretical method, providing atomistic-level details to macroscopic observations. Through this work we will gain a mechanistic understanding of the Cs-clay adsorption process and we will help inform the choice of natural clay between the local naturally available ones, on the nuclear waste disposal sites.

### Main responsibilities

#### Activities:

- Set up MD simulations of systems containing montmorillonite and vermiculite with Cs-137;
- Run MD simulations on a high-performance computer (HPC);
- Evaluate when the simulation is representative of the macroscopic phenomena;
- Analyse simulations to obtain static and dynamic data;
- Learn about chemical mechanisms of ion adsorption by silicate clay minerals;
- Reflect on potential further studies and on the limitations of the used methodology.

### Learning Outcomes

- Learn how to setup and run MD simulations on HPC;
- Gain experience in analysing and interpreting simulation data;
- Understand the theoretical background of MD and how it can be used to explain macroscopic observables;

- Describe the interactions between clay and ions, identify key physiochemical properties of clays for the successful adsorption.

## Knowledge Skills and Experience

Person specification

**Essential:** knowledge of geochemistry, desire to learn processes occurring at molecular level.

**Desirable:** experience with Linux and Python.

## Key contacts

- Dr Valentina Erastova (group leader)
- Hannah Pollak (PhD student mentor)

## Dimensions

This is a 6-week placement with flexible start date between 14 June and 19 July 2021.

**Closing date:** 19 May 2021

**Interview date:** to be determined by the supervisor

**Start date:** flexible start date between 14 June and 19 July 2021

**Hours per week and preferred pattern/restrictions (if applicable):** 35 hours per week (part-time option available)

**Length of internship:** 6 weeks

## Additional Information

### Host and Project outline

The caesium-137 radioisotope is one of the most common fission products of uranium, it is highly soluble and chemically reactive, decaying through high-energy pathways with a half-life of 30 years. These properties make it a dangerous isotope, remaining as a legacy of nuclear catastrophes.

The nuclear accident of Chernobyl (1986) and Fukushima (2011) nuclear power plant has led to the release of large quantities of radioactive Cs-137 into the environment. It was found that the Cs sorption behaviour of the clay materials present in the soil around the site varied greatly. Interestingly, between the two very similar smectite clays, the least amount of Cs was sorbed by montmorillonite and the most by vermiculite. [1]

Within this work we will investigate the adsorption of Cs-137 onto montmorillonite and vermiculite clays at atomic-level resolution. To this end, we will use molecular dynamics (MD) simulations, a theoretical method, providing atomistic-level details to macroscopic observations. Through this work we will gain a mechanistic understanding of the Cs-clay adsorption process.

Smectites are swelling clays with high cation exchange capacity, allowing them to retain radioactive cations, such as Cs and Sr, making them excellent buffer material. [2] In fact, at the nuclear waste disposal sites bentonite, rich in smectites, is used to seal the nuclear waste. Therefore, through this work, we will help inform the choice of natural clay between the local naturally available ones.

Furthermore, if the student progresses rapidly through the study of two aforementioned clays, the project could be extended to kaolinite, a non-swelling clay and a corrosion product of smectites. [2,3]

ACTIVITY: WEEK:	1	2	3	4	5	6
Start in the group, learn using BASH*, background reading on nuclear waste disposal and contamination	X					
Work through MD tutorials*, set-up and run simple test system, visualisation and analysis; reading about MD simulations		X	X			
Getting familiar with HPC Eddie (queuing system, job submissions, scripts for job control on the HPC)			X			
Setup and run simulations with the two clay models				X	X	
Systems analysis, data presentation					X	
Comparison of models to experimental data, discussion					X	X
Conclusion of the project, presentation, short report						X

\*Training will be supported by the tutorials at [erastova.xyz/teaching](http://erastova.xyz/teaching)

[1] Mukai, H., Hirose, A., Motai, S. et al. Cesium adsorption/desorption behavior of clay minerals considering actual contamination conditions in Fukushima. Sci Rep 6, 2016.

[2] Bergaya, Faïza, and Gerhard Lagaly. Handbook of clay science. Newnes, 2013.

[3] Righi, D., Terribile, F. & Petit, S. Pedogenic Formation of Kaolinite-Smectite Mixed Layers in a Soil Toposequence Developed from Basaltic Parent Material in Sardinia (Italy). Clays Clay Miner. 47, 1999.

## Training

Provided Training:

- Introduction to working on a Linux computer;
- Introduction to BASH and Python scripting for simulation setup and submission and data analysis;
- Introduction to using VMD for simulation data visualisation;
- Tutorials for setting up and running MD simulations.

## Budget

£450 Research Costs (included) for Computing time and data storage costs

## Location

Depending on future Covid-19 restrictions, the placement will be held either remotely or at the Joseph Building of the University of Edinburgh's King's Buildings Campus. The student will be provided with a Linux desktop with NVIDIA GPU, allowing fast testing, analysis of the results, and data visualisation. The same computing resources will be available (via VPN and remote login) to the student if they are required to work from home. In this case, the student will need to have access to a computer with stable internet connection.

## Covid-19 contingency plan

This is a computational project, all work can be carried out remotely.

## Programme Information

Research Experience Placement is a summer placement scheme funded by NERC, aimed at undergraduate students to address demographic and diversity-related challenges in the environmental sciences as well as thematic skills gaps (e.g. quantitative skills).

**Please see the application instructions and selection process on the REP webpage: [Research Experience Placements \(REPs\) | The University of Edinburgh](#)**

[Employ.ed on Campus](#) is run by the Careers Service in collaboration with University departments and Schools. It offers exclusive summer internships at the University over the summer for 2nd year to penultimate year undergraduate students studying in an UK Higher Education institution.

As well as great work experience, the Careers Service provides supporting resources, this is combined with a framework to support the development of participants' employability and self-reflection with an [Edinburgh Award](#) as part of the internship.

## Application Support

For guidance on writing an effective application see our website: [CV, Applications and Interview Advice](#)

You can also make an appointment with a Careers Consultant using [MyCareerHub](#).

## Eligibility

Students are subject to eligibility criteria to be able to apply for NERC REPs and must:

- Be undertaking their first undergraduate degree studies (or integrated Masters)
- Be applying for a placement in a different department to their undergraduate degree
- Be eligible for subsequent NERC PhD funding, i.e. be either:
  - an UK citizen OR
  - an EU citizen with pre- or settled status under the EU Settlement Scheme OR
  - a non-EU citizen who have obtained the right to remain in the UK - known as 'indefinite leave to remain' (ILR) O
  - an International/EU student already studying in the UK and currently under a Tier 4 or Student Route Visa with validity until at least September 2021

**REPs do not meet the requirements for a visa request therefore non-UK students who are not currently living in the UK or who are without a suitable UK visa are not eligible to apply.**

Internships are ONLY open to 2nd year to penultimate year undergraduate students studying in an UK Higher Education institution and based in the UK. You cannot take part if you are a visiting student, or you have already taken part in the programme before.

## Privacy Statement

In addition to the University's HR data privacy statement, please read the [Student and Graduate Privacy Statement: Internships and work experience programmes](#) to understand how and why we will use the information you submit for the Employ.ed Programmes

## Health & Safety Requirements for the role

None required

## Key Job hazard information specific to the role

N/A

If you require this document in an alternative format please contact Internships and Work Experience Team by email at [employ.ed@ed.ac.uk](mailto:employ.ed@ed.ac.uk)