

# Computational Techniques in Chemistry

## Session 4: Projects

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Big thanks to Matteo Degiacomi ([matteo.degiacomi@ed.ac.uk](mailto:matteo.degiacomi@ed.ac.uk)) and  
Hannah Pollak ([h.pollak@sms.ed.ac.uk](mailto:h.pollak@sms.ed.ac.uk)) for material development

# Course organisation

	Monday/Tuesday	Thursday/Friday
Week 1	<b>Introduction to Linux and command-line</b>	
	Workshop	Drop-in
Week 2	<b>Introduction to molecular dynamics simulations</b>	
	Workshop	Drop-in
Week 3	<b>Molecular simulation set up of system with an interface or a protein system</b>	
	Workshop	Drop-in
Week 4	<b>Beginning of the individual projects</b>	
	Workshop	Drop-in
Week 5	<b>Drop-in</b>	
	<b>Project Submission</b>	

# Projects

- 30% of the Research Techniques Course
- Each project is unique – you will get your project today
- The project is similar to the work in Session 3
- **You must carry out your project work independently**

# Use of AI

- Allowed, **but must be declared:**
  - What tool has been used (e.g., University-licenced ELM ← recommended);
  - What was the exact prompt;
  - Link to the output ('link to chat' for ChatGpT) or a compilation of outputs as an appendix;
  - What modifications have been done to the generated output before it was incorporated into the submitted work.
- Undeclared use of AI will be flagged as misconduct and treated as plagiarism.

# Project Report Structure

## Abstract

Up to 150 words

- concise summary of your work
  - understandable as a standalone piece

## Methods

~500 words

- all key steps to prepare, run and analyse the simulation
- another scientist must be able to repeat your work

## Conclusions

~100 words

key conclusions from your study

## Introduction

Up to 150 words

motivation for your work

## Results & Discussion

~500 words

- your data
- plots, renderings, tables to support your observations
  - small discussion

## Bibliography

use Mendeley/Endnote/.bib

# Project Report Structure

## System Setup

- structures
- how you assembled the system
- force fields

## Simulation Protocol

- energy minimisation, equilibration, and production runs
- time step and duration
- temperature, pressure

## Analysis

- checks for equilibration
- what part of trajectory used
- analysis
- software used
- how did you plot and render

## Methods

~500 words

- all key steps to prepare, run and analyse the simulation
- another scientist must be able to repeat your work

## Results & Discussion

~500 words

- your data
- plots, renderings, tables to support your observations
- small discussion

## Conclusions

~100 words

key conclusions from your study

- What were your observations?
- Support them with figures (renderings, plots) and tables.
- Captions need to be descriptive, so no need to read the main text.
- Don't forget to state what color is what atom.
- Discuss the findings and compare to the literature.

# Example report

## Investigation of effects of cations on adsorption of decanoic acid by montmorillonite clay

Lisa Simpson s0123456

31 January 2025

### Abstract

This report investigates the role of charge-balancing cations in the adsorption of oil molecules onto smectite clay minerals. Using molecular dynamics simulations, the study examines the adsorption mechanisms of deprotonated decanoic acid on clay surfaces in the presence of sodium ( $\text{Na}^+$ ) and calcium ( $\text{Ca}^{2+}$ ) ions. The results indicate that divalent ions enhance adsorption, compared to monovalent ions. This is attributed to the ability of divalent cations to form cationic bridges between the negatively charged carboxylate group of decanoic acid and the negatively charged montmorillonite clay surface, leading to stronger adsorption interactions.

### Introduction

The adsorption of organic molecules onto soil-forming mineral surfaces plays a crucial role in various natural and industrial processes, including oil recovery, soil chemistry, and environmental remediation. Understanding how charge-balancing cations present in the soils influence adsorption mechanisms is essential for predicting molecular behaviour in complex environmental systems. This study focuses on the adsorption of decanoic acid onto smectite clay in the presence of monovalent sodium ( $\text{Na}^+$ ) and divalent calcium ( $\text{Ca}^{2+}$ ) ions. By using molecular dynamics simulations, we aim to obtain atomistic details of clay-oil interactions, obtaining mechanistic and quantitative information on the underlying processes.

### Methodology

#### System Setup

The clay used in this study is representative of montmorillonite (MMT), with unit cell stoichiometry of  $[\text{Al}_3\text{Mg}][\text{Si}_4\text{O}_{10}](\text{OH})_2$ . The substitution of octahedral  $\text{Al}^{3+}$  for  $\text{Mg}^{2+}$  gives rise to the negative layer charge, which is charge-balanced by positive cations  $\text{Na}^+$  or  $\text{Ca}^{2+}$ . These cation-clay systems are named Na-MMT and Ca-MMT, respectively. The pKa of decanoic acid is 4.9, i.e., at pH > 4.5 decanoic acid is deprotonated to form carboxylate anions,  $\text{CH}_3(\text{CH}_2)_8\text{COO}^-$ .

The clay unit cell with the size of  $0.5160 \text{ nm} \times 0.8966 \text{ nm} \times 0.9347 \text{ nm}$  in  $x$ ,  $y$ ,  $z$  directions was replicated  $7 \times 6 \times 1$  times, to form a layer in  $xy$ -plane of  $3.62523 \text{ nm} \times 5.39930 \text{ nm}$ . The simulation box was then expanded in the  $z$ -direction to be approximately 10 nm, where the clay layer occupied the region of  $0 < z < 1 \text{ nm}$ . Subsequently, 11 deprotonated decanoic acid molecules were inserted into the

1

yellow, Al - cyan, Mg - pink,  $\text{Na}^+$  - cyan spheres,  $\text{Ca}^{2+}$  - blue spheres,  $\text{Cl}^-$  - green spheres, for clarity water may be shown as a transparent surface.

2

The system was solvated, by the box. Any water molecules were removed. The ions were and ionic concentration of 0.1 M. ions and Ca-MMT system with

old,<sup>1</sup> decanoic acid was assigned the SPC model with force field

24.4,<sup>2</sup> with electrostatic and van

convergence achieved once the 0 kJ mol<sup>-1</sup> atom<sup>-1</sup>. Subsequently, size of 1 fs in isothermal-isobaric C and a semi-isotropic C-rescale allows to independently rescale for the layer to compress at a achieving the set pressure. The run with the timestep of 2 fs is the same as for equilibration.

the potential energy, pressure and drifts. For further trajectory- emerged when root-mean-square<sup>2</sup>, water, decanoic acid and ions) as explored the available phase- d was the slowest to level, which before, first 20 ns of production

z-axis, i.e. perpendicular to clay each component in the system. for water and carboxylate group s information on coordination plots are produced with XmolGrace, MD (Visual Molecular Dynamics)

C - grey, H - white, O - red, Si -

### Results and Discussion

Upon visual examination of the systems (Figures 1A and 1B) it became apparent that in both systems, decanoic acid forms a cluster with its hydrophobic chains pointing towards the centre and carboxylate groups exposed to water. Cations surround the deprotonated groups. Furthermore, both  $\text{Na}^+$  (cyan spheres, Figure 1A) and  $\text{Ca}^{2+}$  (blue spheres, Figure 1B) form a layer above the negatively charged surface of the clay. Occasional single molecule of decanoic acid is dispersed away from the cluster (as seen in Figure 1A) but will rapidly return to organic cluster. The biggest difference between two systems is that when a monovalent cation is present the organic cluster remains in the middle of the clay nanopore, not interacting with clay surfaces. In the Ca-MMT system, the divalent cation facilitates interaction between the organics and clay surface. This observation is also confirmed by linear number density profiles (Figures 1C and 1D), that provide a probabilistic representation of the location of each component during whole simulation. In the case of Na-MMT, decanoic acid (red line, Figure 1C) remains in the centre of the simulation box and, therefore, not in contact with the clay surface. In the case of Ca-MMT, decanoic acid peak (red line, Figure 1D) is located next to the clay surface. The cations (blue line, Figures 1C and 1D) are positioned next to the clay surface and, in the case of Ca-MMT, also lay between the organics and the clay.

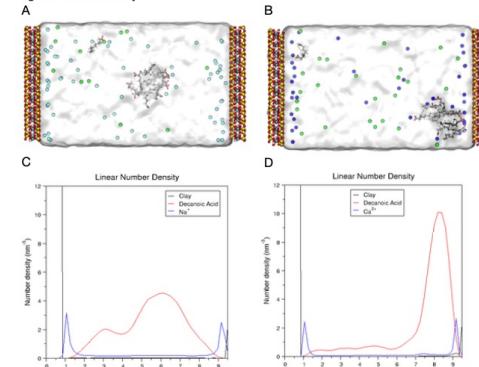


Figure 1: Visualisation of representative configurations of (A) Na-MMT and (B) Ca-MMT systems with deprotonated decanoic acid. Their corresponding linear number densities are given in (C) and (D) respectively.

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Figure 2: Visualisation of representative configurations of decanoic acid bridged by  $\text{Ca}^{2+}$  cations to the surface of MMT.

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### Conclusions

This study details the effect of cations on the adsorption of organic species by clay minerals. In the case of a deprotonated organic species, the presence of divalent ions will enable their adsorption onto the clay surface via a bridging mechanism. This is not possible when charge-balancing ions are monovalent. This work gives insights into the intricate interactions between organic and mineral species in the soil and have implications for the fields of environmental science and engineering.

### References

1. Cygan, R. T., Liang, J. J. & Kalinichev, A. G. Molecular models of hydroxide, oxyhydroxide, and clay phases and the development of a general force field. *Journal of Physical Chemistry B* **108**, 1255–1266 (2004).
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3. Van Der Spoel, D. et al. GROMACS: Fast, flexible, and free. *J Comput Chem* **26**, 1701–1718 (2005).
4. Humphrey, W., Dalke, A. & Schulten, K. VMD -- Visual Molecular Dynamics. *J Mol Graph* **14**, 33–38 (1996).
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6. Li, M., Duan, Z., Zhang, Z., Zhang, C. & Weare, J. The structure, dynamics and solvation mechanisms of ions in water from long time molecular dynamics simulations: a case study of  $\text{CaCl}_2$  (aq) aqueous solutions. *Mol Phys* **106**, 2685–2697 (2008).
7. Underwood, T., Erastova, V., Cubillas, P. & Greenwell, H. C. Molecular dynamic simulations of montmorillonite organic interactions under varying salinity: An insight into enhanced oil recovery. *Journal of Physical Chemistry C* **119**, 7282–7294 (2015).

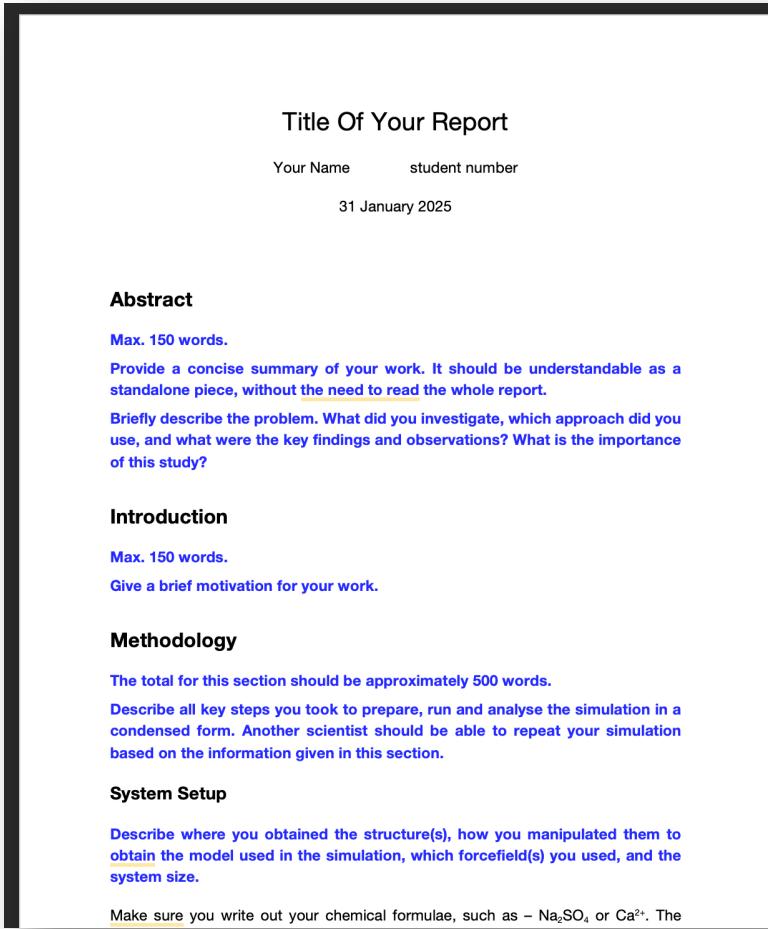
5

# Templates

- Word.doc

- OverLeaf – LaTeX format [LINK](#)

<https://www.overleaf.com/read/vhpwvtgwygbx#cb9c81>



The screenshot shows the PgT\_CompChem software interface with a LaTeX template for a report. The left sidebar displays files: main.tex (selected), my\_plot.png, my\_rendering.png, and references.bib. The file outline shows sections: Abstract, Introduction, Methodology (expanded to System Setup, Simulation Protocol, Analysis), Results and Discussion, and Conclusions. The code editor contains the LaTeX source code for the report, including sections for Title, Abstract, Introduction, Methodology, and System Setup. The right panel shows the rendered document with sections for Title, Abstract, Introduction, Methodology, and System Setup.

PgT\_CompChem\_Template\_2025

Code Editor Visual Editor Normal text B I Ω ... Recompile

main.tex

my\_plot.png

my\_rendering.png

references.bib

File outline

- Abstract
- Introduction
- Methodology
  - System Setup
  - Simulation Protocol
  - Analysis
- Results and Discussion
- Conclusions

```
22 \title{Title of Your Report}
23 \author{Your Name \textbf{and} student number}
24 \date{\today}
25
26 \begin{document}
27
28 \maketitle
29
30 %%%%%% ABSTRACT %%%%%%
31
32 \section*[Abstract]
33
34 \textbf{\color{blue}{Max. 150 words. \\}}
35 Provide a concise summary of your work. It should be understandable as a standalone piece, without the need to read the whole report. \\
36 Briefly describe the problem. What did you investigate, which approach did you use, and what were the key findings and observations? What is the importance of this study?
37 }
38
39 %%%% INTRO %%%%
40
41 \section*[Introduction]
42
43 \textbf{\color{blue}{Max. 150 words. \\}}
44 Give a brief motivation for your work.\\
45
46
47 %%%% METHODOLOGY %%%%
```

Title of Your Report

Your Name student number

February 2, 2025

## Abstract

Max. 150 words.  
Provide a concise summary of your work. It should be understandable as a standalone piece, without the need to read the whole report.  
Briefly describe the problem. What did you investigate, which approach did you use, and what were the key findings and observations? What is the importance of this study?

## Introduction

Max. 150 words.  
Give a brief motivation for your work.

## Methodology

The total for this section is approx. 500 words.  
Describe all key steps you took to prepare, run and analyse the simulation in a condensed form. Another scientist should be able to repeat your simulation based on the information given in this section.

## System Setup

Describe where you obtained the structure(s), how you manipulated them to obtain the model used in the simulation, which forcefield(s) you used, and the system size.



# FEEDBACK PLEASE!



- 1 – go to [wooclap.com](https://wooclap.com)
- 2 – event code **EUCRND**