Università degli Studi di Napoli Federico II

SCUOLA POLITECNICA E DELLE SCIENZE DI BASE

Corso di Laurea Magistrale in Fisica

Master's Thesis

Properties of molecular crystals using machine learning potentials

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Acknowledgments

I would like to thank you for using my template and the team of typst for the great work they have done and the awesome tool they developed. Remember that it's best practice to thank the people you worked with before thanking your family and friends.

Abstract

Molecular crystals play an important role in the field of materials science, particularly in drug development, electronics, and renewable energy sectors.

In this work we will study the properties of molecular crystals, using recently developed Machine Learning potentials to model their behaviour and characteristics. We will be primarily focusing on water as the initial subject, followed by a study of a selection of other molecular crystals.

Traditional approaches often grapple with the trade-off between computational expense and accuracy. The application of Machine Learning potentials captures complex intermolecular interactions with a significantly reduced computational cost compared to traditional ab-initio methods.

We will study the capabilities of trained Machine Learning potentials to accurately predict lattice energies, polymorphic behaviours, and response to external conditions like temperature and pressure. We will also study dynamic properties such as phonon spectra to complete the insight into the physical and chemical behaviours of molecular crystals.

CONTENTS

1 Introduction

Remeber that this is not only a repeat of the abstract, the introduction should be a more detailed explanation of the problem and the background of the study. If we want to reference an element in the bibliography you can do so like this [1].

2 Example

This is an example chapter [2], Lorem ipsum dolor sit amet, consectetur adipiscing elit, sed do eiusmod tempor incididunt ut labore et dolore magnam aliquam quaerat voluptatem. Ut enim aeque doleamus animo, cum corpore dolemus, fieri tamen permagna accessio potest, si aliquod aeternum et infinitum impendere malum nobis opinemur. Quod idem licet transferre in voluptatem, ut postea variari voluptas distinguique possit, augeri amplificarique non possit. At etiam Athenis, ut e patre audiebam facete et urbane Stoicos irridente, statua est in quo a nobis philosophia defensa et collaudata est, cum id, quod maxime placeat, facere possimus, omnis voluptas assumenda est, omnis dolor repellendus. Temporibus autem quibusdam et.

```
// This is a block of code

#include <stdio.h>

int main() {
  printf("Hello, World!");
  return 0;
}
```

- And this
- Is a list
  - With a sublist

Now an equation:

$$\sum_{k=1}^{n} k = \frac{n(n+1)}{2} \tag{1}$$

2.a With a Section

This is a section, Lorem ipsum dolor sit amet, consectetur adipiscing elit, sed do eiusmod tempor incididunt ut labore et dolore magnam aliquam quaerat voluptatem. Ut enim aeque doleamus animo, cum corpore dolemus, fieri tamen permagna accessio potest, si aliquod aeternum et infinitum impendere malum nobis opinemur. Quod idem licet transferre in voluptatem, ut postea variari

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2.a.I And a Subsection

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3 Conclusions

A good conclusions chapter really helps to tie up the whole thesis.

REFERENCES

[1] "UniTO typst template." [Online]. Available: https://github.com/eduardz1/UniTO-typst-template

[2] "Typst." [Online]. Available: http://typst.app/

[3] Thomas H. Cormen, Charles E. Leiserson, Ronald L. Rivest, and Clifford Stein, *Introduction to Algorithms, Third Edition*, 3rd ed. MIT Press, 2009. doi: 10.5555/1614191.