

NeNa

Untertitel

Projektarbeit

im Fachbereich Physik



TECHNISCHE
UNIVERSITÄT
WIEN

vorgelegt von: Gabriel Sommer

Studiengang: Physik

Matrikelnummer: 11912404

Prüfer: Andreas Grüneis

July 16, 2025

Zusammenfassung

Zugsamenfassung: Ziel, Methoden, Ergebnisse, Schlussfolgerungen

Contents

List of Figures	III
List of Tables	IV
Listings	V
Abkürzungsverzeichnis	VI
Symbolverzeichnis	VII
1 Einleitung	1
2 Aufgabenstellung	2
3 Theory	3
3.1 Statistical Mechanics	3
3.2 Relaxation in LAMMPS	4
3.3 Simulated Annealing	4
3.4 Symmetry optimization	5
3.5 DFT optical spectra	5
4 Neon interaction LAMMPS setup	7
5 Finding Minima of neon replacements	8
5.1 Sodium Monomer	8
5.2 Sodium Dimer	8
6 DFT optical spectra results	9
7 Erstes Kapitel	10
7.1 Einrichten dieser Vorlage	10
7.2 Drucken	10
7.3 Text	10
7.4 Bilder	11
7.5 Programmcode	11
7.6 Tabellen	11
7.7 Zitieren	12
7.8 Abkürzung	12
7.9 Aufzählungen	12

7.10	Referenzieren	13
7.11	Textstyle	13
7.12	Formeln	13
7.13	Sections	13
8	Ausblick	14
	Bibliography	i
A	Anhang	ii
A.1	Inhalt des beigefügten Datenträgers	ii

List of Figures

3.1	state evolution $(\vec{\mathbf{q}}(t), \vec{\mathbf{p}}(t))$ through $6N$ -dimensional phase space	4
5.1	Brute force for single sodium atom	8
7.1	Placeholder Image	11

List of Tables

7.1 Placeholder table	12
---------------------------------	--------------------

Listings

3.1	Simulated annealing algorithm	5
3.2	lexicographically sorting point group symmetries	6
7.1	Code Placeholder	11

Abkürzungsverzeichnis

API	Application Programming Interface
LAMMPS	Large-scale Atomic/Molecular Massively Parallel Simulator

Symbolverzeichnis

Symbol	Bedeutung	Einheit
B	magnetische Flussdichte	T
D	Elektrische Flussdichte	A s m^{-2}

1 Einleitung

Einleitung: Wieso sollte diese Arbeit gelesen werden?

2 Aufgabenstellung

We are here trying to calculate optical absorption spectra with vasp. The atomic configuration is a cavity inside a neon crystal that was proposed to be filled with either a single sodium atom or two sodium atoms (a sodium dimer). Now the first step was to find configurations of cavities, i.e. how many neon atoms will be replaced by an inserted sodium atom and subsequently by a sodium dimer. This substitution number will be denoted as S in the following thesis. For these specific configurations the optical absorption spectra will be calculated and compared with the experiment.

3 Theory

3.1 Statistical Mechanics

First we consider the system of the crystal of Neon Atoms as a canonical ensemble, this means it will be described under the assumption of an infinitely large heat bath by Boltzmann statistics. The probability distribution of members of the ensemble will then be

$$p(\vec{\mathbf{q}}, \vec{\mathbf{p}}) = \frac{e^{-\beta H(\vec{\mathbf{q}}, \vec{\mathbf{p}})}}{\int \dots \int e^{-\beta H(\vec{\mathbf{q}}, \vec{\mathbf{p}})} d^{3N} \vec{\mathbf{q}} d^{3N} \vec{\mathbf{p}}}, \quad (3.1)$$

with N being the number of particles.

Now an ensemble is to be understood as many fictional copies of the same system representing the states that a system will explore when propagating in time according to Hamilton's equation of motion. The ensemble distribution represents the relative number of times that an ergodic system will come by a given state after an infinite amount of time has passed. Now for a crystal in principle this still holds. At low temperatures though the phase space that is being explored can be abstracted in such cases. The reason is that the system will for a given finite time usually explore only nearby points in the phase space. This is the crystal configuration but allowing for dynamics such as lattice vibrations and thermal movement of the atoms with respect to their lattice site. So for a given initial point in phase space the system will mostly explore its proximity until it probabilistically jumps to another volume of phase space whose proximity then will be explored for some further time. Now this means the systems lattice configuration has changed which at low but non zero temperature should be reasonable. We now consider these volumes of phase space (being approximately confined regions, i.e. configurations of e.g. a crystalline structure) to be discrete states that the system can be in. So our canonical distribution now is a discrete one, each state representing such a configuration volume. What's left is to figure out what state of the still continuously possible states inside will be used to represent each configuration. We in this work will use the state $(\vec{\mathbf{q}}_{0i}, \vec{\mathbf{p}}_{0i})$ that locally minimizes $H(\vec{\mathbf{q}}, \vec{\mathbf{p}})$. Such a minimum can be found by employing a relaxation calculation in Large-scale Atomic/Molecular Massively Parallel Simulator ([LAMMPS](#)). The Boltzmann distribution now follows to be:

$$p(\vec{\mathbf{q}}_{0i}, \vec{\mathbf{p}}_{0i}) = \frac{e^{-\beta H(\vec{\mathbf{q}}_{0i}, \vec{\mathbf{p}}_{0i})}}{\sum_n e^{-\beta H(\vec{\mathbf{q}}_{0n}, \vec{\mathbf{p}}_{0n})}}. \quad (3.2)$$

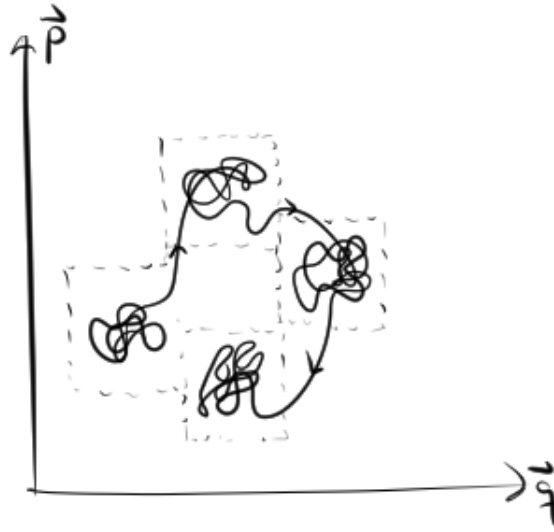


Figure 3.1: state evolution $(\vec{q}(t), \vec{p}(t))$ through $6N$ -dimensional phase space

grand canonical ensemble with two chemical components

sub term of grand canonical ensemble with only $ne1$ and $ne2$

Explanation for cohesive energy

3.2 Relaxation in LAMMPS

relaxation theory form lammmps described in [1] Bitzek, Koskinen, Gahler, Moseler, Gumbusch, Phys Rev Lett, 97, 170201 (2006). Testcite Griffiths[2]

3.3 Simulated Annealing

The object that is being annealed is a state vector containing binary information for every lattice site. It refers to the ideal static lattice of the neon structure. A positive value or 1 refers to an atom being present in the initial structure and a negative value or 0 means the neon atom is vacant at this site. So every digit of the binary state refers to a certain specific lattice site. The energy functional of the annealing process will be the energy after minimization (i.e. relaxation) of the above described state vector. This state vector therefore refers to an initial pre-relaxation configuration where sites are simply removed with [LAMMPS](#).

Energy functional contains cohesive Energy/chemical potential, not just hamiltonian!!

Listing 3.1: Simulated annealing algorithm

```
1 stateVector = [1,1,1,1,1,1,1,1,1,1,1,1,1,1]
2 alpha = (Tend / Tstart) ** (1 / N)
3
4 for i in N:
5     T = Tstart * (alpha**i)
6
7     n = randomInt(1,len(stateVector))
8     stateVector[n] = 1 - stateVector[n]
9
10    stateVectorOld = stateVector
11
12    EOld = minimizeEnergy(stateVectorOld)
13    E = minimizeEnergy(stateVector)
14
15    if E >= EOld:
16        stateVector = stateVectorOld
17    elif random(0,1)<=exp(-1/T*(E-EOld)):
18        stateVector = stateVectorNew
19
20 S = 1
21 for site in stateVector:
22     if site == 0:
23         S += 1
```

3.4 Symmetry optimization

In the case of a single sodium atom inserted in the neon crystal the highly symmetrical structure was exploited to reduce redundant minimization calls in the annealing routine, by identifying symmetrically equivalent structures and caching them. Applying rotation and reflection matrices of the octahedral symmetry group to a single configuration was used to quickly create all equivalent configurations. By sorting them lexicographically and picking e.g. the first, one ensures every redundant set of configurations is always represented by the same configuration.

3.5 DFT optical spectra

Listing 3.2: lexicographically sorting point group symmetries

```
1 equivs = np.transpose(np.einsum("klj,ij", oh_group, pos), (1, 0, 2))
2
3 for k in range(equivs.shape[0]):
4     equivs[k] = equivs[k][np.lexsort(equivs[k].T[:,-1])].copy()
5     sorting_idx = np.lexsort(
6         np.transpose(equivs, (2, 1, 0)).reshape(pos.size, oh_group.shape[0])
7     )
8     pos = equivs[sorting_idx[0], :, :]
```

4 Neon interaction LAMMPS setup

- potential curves for na-ne, na-na, ne-ne interactions
- explain setup of calculation with ball being carved out
- maybe here explain the nearest neighbours

5 Finding Minima of neon replacements

5.1 Sodium Monomer

- Not feasible to brute force dimer with 3rd nearest neighbors
- explain nearest neighbors
- explain confirmation of algorithm with brute force for mono sodium
- explain how plot is created with sweeps
- more complicated symmetries
- compare figures
- calculation for dimer
- discuss noteworthy structure (e.g. inner shell carved out)

Now first by brute force search we know the minima for a single sodium atom.

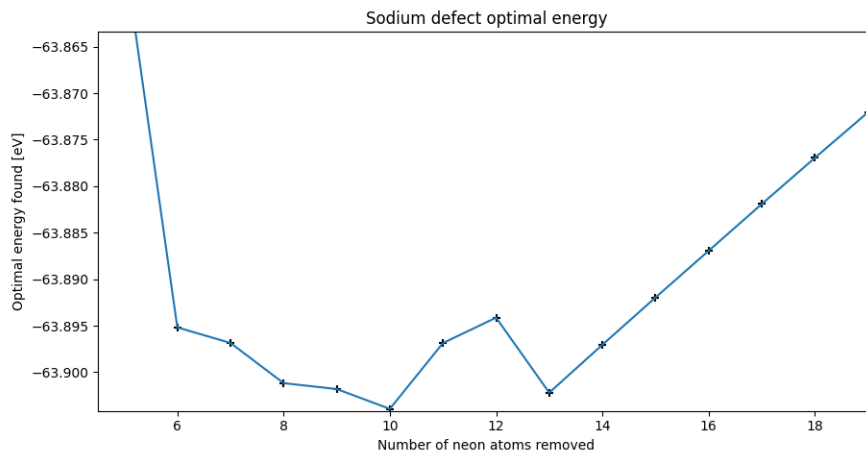


Figure 5.1: Brute force for single sodium atom

5.2 Sodium Dimer

- maybe think about symmetry
- same graphics as for the monomer case
- heuristically take the maxima of these plots
- give structures
- discuss structures (inner shell carved out)

6 DFT optical spectra results

Zweites Kapitel

7 Erstes Kapitel

7.1 Einrichten dieser Vorlage

→ Füge in der *main.tex* alle relevanten Metainformationen wie Titel, Autor, ... usw. ein.

→ Ersetze das Logo in *Inhalt/Bilder/logo.png* mit dem passenden Logo und passe ggf. den Dateinamen und -endung in *Sonstiges/Titelblatt.tex* an

→ Passe den Anhang in *Verzeichnisse/Anhang.tex* entsprechend an.

7.2 Drucken

In der *main.tex*:

- oneside in twoside ändern
- openright einkommentieren
- Den Befehl `\myemptypage` hinter dem Titelblatt einkommentieren

In *Config/Packages.tex*:

- alle farblichen links im hyperref package auskommentieren

In *Config/Seitenstil.tex*:

- pagemark von `\cfoot{}` in `\ofoot{}` tauschen

7.3 Text

Lorem ipsum dolor sit amet, consectetur adipiscing elit. Nullam placerat, dui ac vulputate commodo, est mi sagittis ipsum, sed ullamcorper nunc mauris eu sem. Vestibulum egestas, eros eu rhoncus suscipit, tortor diam molestie libero, in aliquam nisl lectus in dui. Quisque aliquet metus ut nisi volutpat, in hendrerit lectus porta. Etiam efficitur elit purus, vitae fringilla elit tempor ac. Aenean nec ipsum dictum, fringilla lectus a, aliquam neque. Nulla nec ante ut lectus sollicitudin elementum quis ac mi. Praesent a tellus magna.

Cras eget nulla dignissim, dictum libero non, consectetur elit. Nulla felis lorem, consequat sit amet interdum non, tincidunt eget leo. Integer mollis fringilla elit sit amet posuere. Fusce porttitor massa augue, ut faucibus risus lobortis at. Quisque lacinia erat in cursus sodales.

Donec aliquam lorem feugiat nibh dapibus, at blandit erat pretium. Aliquam erat volutpat. Quisque tempus dui at augue aliquet mattis. Aliquam erat volutpat.

7.4 Bilder

Bilder in dem Ordner *Inhalt/Bilder* hinterlegen.



Figure 7.1: Placeholder Image

7.5 Programmcode

Programmcode in dem Ordner *Inhalt/Code* hinterlegen.

Listing 7.1: Code Placeholder

```
1 print("hello world!")
```

7.6 Tabellen

[Zum einfacheren erstellen von Tabellen](#)

Table 7.1: Placeholder table

Spalte 1	Spalte 2
a	1
b	2
c	3

7.7 Zitieren

Hier ein einfaches Zitat [3].

Bibliographie Einträge in *Verzeichnisse/Literatur.bib* hinterlegen.

7.8 Abkürzung

Abkürzungen in dem Ordner *Verzeichnisse/Abkürzungsverzeichniss.tex* hintelegen.

Beim ersten Verwenden wird die Abkürzung ausgeschrieben, beim zweiten mal wird nur die Abkürzung benutzt.

Erste Verwendung: Application Programming Interface ([API](#))

Zweite Verwendeung: [API](#)

7.9 Aufzählungen

Normale Aufzählung:

- Stichpunkt 1
- Stichpunkt 2
- Stichpunkt 3

Aufzählung mit custom Symbolen:

- xyz Stichpunkt 1
- abc Stichpunkt 2
- ! Stichpunkt 3

7.10 Referenzieren

Eine Referenz zu unserem Bild [7.1](#)

Eine Referenz zu unserer Tabelle [7.1](#)

Eine Referenz zu der Section Bilder [7.4](#)

7.11 Textstyle

Kursiver Text

Bold Text

`Mono Spaced Text` (Für bsp. Programmcode)

7.12 Formeln

[Referenz für Mathematik in Latex](#)

$$\Gamma_I = \sigma(W_I[h_t|X_t]) \quad (\text{Input Gate}) \quad (7.1)$$

$$\Gamma_O = \sigma(W_O[h_t|X_t]) \quad (\text{Output Gate}) \quad (7.2)$$

$$\Gamma_F = \sigma(W_F[h_t|X_t]) \quad (\text{Forget Gate}) \quad (7.3)$$

Symbolbeschreibungen werden in dem Symbolverzeichnis unter *Verzeichnisse/Symbolverzeichnis.tex* hinterlegt.

So werden Formeln im Text angegeben x^2 und so kann man im Text einen übersichtlicheren Bruch verwenden $kg\,m/s^2$.

7.13 Sections

7.13.1 subsection

subsubsection

8 Ausblick


Ausblick

Bibliography

- [1] P. Bitzek et al. “Structural Relaxation Made Simple”. In: *Physical Review Letters* 97.17 (2006), p. 170201. DOI: [10.1103/PhysRevLett.97.170201](https://doi.org/10.1103/PhysRevLett.97.170201).
- [2] David J. Griffiths. *Introduction to Quantum Mechanics*. 3rd ed. Cambridge University Press, 2018. ISBN: 9781107189638.
- [3] Autor A, Autor B, and Autor C. “Titel”. In: *Journal* 29.4 (2999), pp. 195–202.

A Anhang

A.1 Inhalt des beigefügten Datenträgers

 Datenträger



A



a



b



c



B



a



b



A

Eidesstattliche Erklärung

Ich, Gabriel Sommer, versichere hiermit, dass ich die vorliegende Arbeit selbstständig verfasst und keine anderen als die angegebenen Quellen und Hilfsmittel benutzt habe, wobei ich alle wörtlichen und sinngemäßen Zitate als solche gekennzeichnet habe.

Diese Arbeit wurde bisher in gleicher oder ähnlicher Form keiner anderen Prüfungsbehörde vorgelegt und auch nicht veröffentlicht.

Vienna, den July 16, 2025

GABRIEL SOMMER

Declaration of Authorship

I, Gabriel Sommer, hereby declare that I have written the present thesis independently and have used no sources or aids other than those explicitly stated. All direct quotations and all paraphrased ideas have been clearly marked as such.

This work has not been submitted, either in the same or a substantially similar form, to any other examination board, nor has it been published elsewhere.

Vienna, July 16, 2025

GABRIEL SOMMER