



Artificial Intelligence for Materials Science (AiMat) Group
 Institute of Theoretical Informatics (ITI)
 Karlsruhe Institute of Technology (KIT)

Supervision of Bachelor and Master theses projects (as of January 2023)

Phase	Required steps	Optional steps	Time frame
0. Study	- You obtain basic knowledge in programming (python) and in the field of machine learning	- You attend one of the seminars of the AiMat Group For MA: - You attend the lecture " Machine Learning for Natural Sciences " by Pascal Friederich and participate in the tutorial - You participate in " Praxis der Forschung " as ideal preparation for a research-oriented thesis	1-2 years
1.1 Contacting	Email to Pascal Friederich (pascal.friederich@kit.edu) or potential supervisors (see https://aimat.science) - Mention previous experience in Machine Learning and programming - Mention prior knowledge of chemistry/material science, if applicable.		Ideally at least 2-3 months before the desired start of work
1.2 Finding topics	- We suggest topics , you think about them, add your own thoughts, we discuss them together and agree on a topic for the next step	- You read about possible topics in the AiMat research group (website, publications, etc.) - You propose one or more topics/directions from our group research - As an overview and source of inspiration, the publications of recent years may be useful (https://scholar.google.com/citations?user=3B5h6u0AAAAJ) - You can also suggest your own topics beyond the work of the group	2-3 weeks
1.3 Exposé	You describe the following points on 2-3 pages (in English): - General topic and motivation - Relevant literature - Scientific question - Objectives of the work (both mandatory objectives and optional additional objectives) - Concrete work steps - Time planning for the next 4/6/12		2-3 weeks

	<p>months (Info BA/Info MA/Physics MA)</p> <p>Please share an editable (overleaf) document with your supervisor for feedback and comments.</p> <p>The time to prepare the exposé is not part of the thesis project duration.</p>		
1.4 Registration	<p>They send information to the secretary, Stephanie Wolf (stephanie.wolf@kit.edu, Pascal in cc):</p> <ul style="list-style-type: none"> - Name - uxxxx abbreviation - Matrikelnummer - Desired registration date - BA/MA - Preliminary title of the paper (in English, note capitalization) <p>The registration date will be shifted in case of planned holidays during the thesis project and in case of planned exams (e.g. by one week per exam). The actual time to work full-time on the thesis should be 4/6/12 months (depending on the study program).</p>		At least one week before desired registration date
1.5 Check-in for BA/MA students	<p>You contact Tobias Schlöder to complete the formal check-in process:</p> <ul style="list-style-type: none"> - Key if necessary - Accounts needed - ... 		After registration
2.1 Implementation	<ul style="list-style-type: none"> - You will meet regularly with your supervisor: <ul style="list-style-type: none"> -- Minimum: Every 4 weeks (but then a short update on Slack at least every 2 weeks). -- Maximum: One formal weekly meeting (closer collaboration is possible). - If you are not directly supervised by Pascal Friederich, arrange at least 3 appointments with him: After about one month, in the middle of the execution, and at the latest 2 weeks before submission. - (All) meetings should be prepared and include (in the form of a presentation, ideally on a collaborative platform such as Google Slides or overleaf): <ul style="list-style-type: none"> -- Brief recap of the last meeting and plans/decisions. -- Overview of the work done -- Presentation of the results -- What worked, what didn't work? -- What are the next steps? -- What are open questions? - Code should be commented, understandable, reproducible, modular, and extensible and stored in a GitHub repository, ideally within aimat-lab 	<ul style="list-style-type: none"> - You are already preparing for the writing phase by: <ul style="list-style-type: none"> -- Design and development of code: Clean, modular, well-documented, and extensible. -- Plan experiments and baselines as systematically as possible and perform them in an automated and reproducible manner. -- Document results, e.g. in the form of presentations and "living" documents. -- Fully automate experiments (data preparation, training, analysis) and data visualization. Always design plots in a "publication ready" (or "thesis ready") way: All axes have labels, no internal notations, as few abbreviations as possible, intuitive, aesthetic, and clear design, etc. -- Document the progress of successes and failures right away in written format. Preserve relevant code and associated data and results and systematically/retrievably - You will work on-site regularly (room 105 in building 40.28, workstations with monitor and docking station are available) to exchange ideas with other group members, participate in group life 	~ 3/5/11 months (Info BA/Info MA/Physics MA)

	<p>accounts: https://github.com/aimat-lab</p> <ul style="list-style-type: none"> - The code needed for the main experiments should be clearly labeled and automated to reproduce the main results of the work. Jupyter notebooks can be used if reproducibility is ensured. 	(lunch, meetings, etc.), come to the group meeting, and thus gain insight into scientific work.	
2.2 Writing the work	<ul style="list-style-type: none"> - You take enough time to write the thesis. The better the preparation and documentation, the more efficient the work will be - Use LaTeX - You start with your own methods, results, and discussion, built around key illustrations/diagrams/figures/tables - After that Introduction and Related Work - After that, summary and outlook (since everything has to be brought together here) - At the very end: Abstract (see Nature Summary paragraph) - A checklist of the most important aspects and evaluation criteria is provided 	- Carefully check the evaluation criteria	~ 1 month
2.3 Delivery	<ul style="list-style-type: none"> - Submission of 2 printed (A4, soft cover, "perfect binding") and signed copies, ideally one day before the deadline (for emergencies). - Make an appointment in advance so that either Pascal Friederich or Stephanie Wolf can receive the work in person - The work is entered as "submitted" in the campus system 		At the latest: One day before the official deadline
2.4 Lecture	<ul style="list-style-type: none"> - You make an appointment for a group meeting presentation with Pascal Friederich, Chen Zhou, and Marlen. - You will present your work in 30-45 minutes, plus discussion and questions 	- You will do a test presentation with your supervisor, approximately one week before the final lecture.	No later than 4 weeks after handing in the thesis
2.5 Grade and feedback	<ul style="list-style-type: none"> - Pascal Friederich prepares a report in consultation with the direct supervisors and determines the grade. Evaluation criteria are available - The grade will be entered into the campus system - You will receive the grade and can schedule a feedback session if needed - You contact Tobias Schlöder for check-out (key return, accounts, etc.) 	- You sign the AiMat guestbook (in case you leave the group after work) 😊	1-3 weeks after the presentation

General information from the Informatics department can be found here:

- https://www.informatik.kit.edu/faq-wiki/doku.php?id=bachelorarbeit_allg
- https://www.informatik.kit.edu/faq-wiki/doku.php?id=masterarbeit_allg