

Master thesis proposal

Machine Learning of Electro-Optical Properties with Graph Neural Networks

Keywords : Machine Learning, Materials Science, Pockels Effect, Graph Neural Networks, Computational Materials Science, Electro-Optics

SCIENTIFIC DESCRIPTION :

This project addresses the significant computational bottleneck in predicting the Pockels tensor – a key material property governing the electro-optical response of materials under the application of a modulating electric field and a laser beam – which currently limits the efficient discovery of materials for telecommunication, advanced photonic and quantum technologies. Traditional approaches rely on computationally intensive ab initio calculations, restricting the scope of materials screening and optimization.

To overcome these limitations, the project proposes a novel data-driven approach leveraging state-of-the-art equivariant Graph Neural Networks (GNNs). Unlike standard GNNs, equivariant architectures are designed to respect the symmetries of physical systems (rotations, reflections, etc.), leading to improved generalization and data efficiency – crucial when modeling properties as complex and costly to compute as the Pockels tensor. These networks will be trained to capture the intricate relationships between atomic structure and electro-optical response.

Predicting the Pockels tensor presents a formidable challenge for both theory and machine learning. It requires accurate treatment of many-body electronic interactions, as well as a deep understanding of the interplay between crystal symmetry and tensorial properties. Moreover, the scarcity of experimental data for Pockels coefficients highlights the need for robust, generalizable machine learning models that can extrapolate beyond limited training sets.

The project will therefore develop a physically informed training strategy, combining symmetry-aware loss functions with advanced data augmentation techniques. The resulting models aim to provide a computationally efficient framework for predicting the Pockels tensor, accelerating the discovery of novel electro-optical materials.

A distinctive feature of this project is its collaborative research environment. The student will work directly with:

- A group at ETH Zurich, internationally recognized for expertise in calculating Pockels tensors and their application in electro-optical devices.
- A group in Bremen, who have developed automated DFT workflows capable of computing Pockels tensors at scale.
- The host group in Grenoble, led by an expert in equivariant neural networks, providing cutting-edge expertise in physics-based machine learning.

This synergy offers the student a unique opportunity to contribute to an active, international research effort tackling an unsolved scientific challenge, while gaining advanced expertise in both quantum materials modeling and modern machine learning methods. Beyond methodological development, the outcomes of this work have the potential to enable the rational design of materials for high-speed optical communications, quantum key distribution, and integrated photonics.



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Techniques/methods in use : This project utilizes equivariant Graph Neural Networks (GNNs) trained on Density Functional Theory (DFT) data to predict Pockels tensors. JAX will enable efficient automatic differentiation for physically-informed machine learning and robust model validation.

Budget description and use : Applicant salary and short research visit to ETH Zurich.

Applicant skills :

This project is suitable for a candidate studying physics, materials science or computer science and will be adapted to emphasise the skills and interests of the chosen candidate.

Skills that are useful to have: materials science, knowledge of atomistic physics, knowledge of Python programming language, machine learning experience, materials modelling

Industrial partnership : N/A

Internship supervisor(s) :

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Virginie de Mestral (ETH Zurich, supervisor Prof. Mathieu Luisier),

Lorenzo Bastonero (University of Bremen, supervisor Prof. Nicola Marzari)

Internship location : SIMaP, Grenoble-INP

Possibility for a Doctoral thesis : No

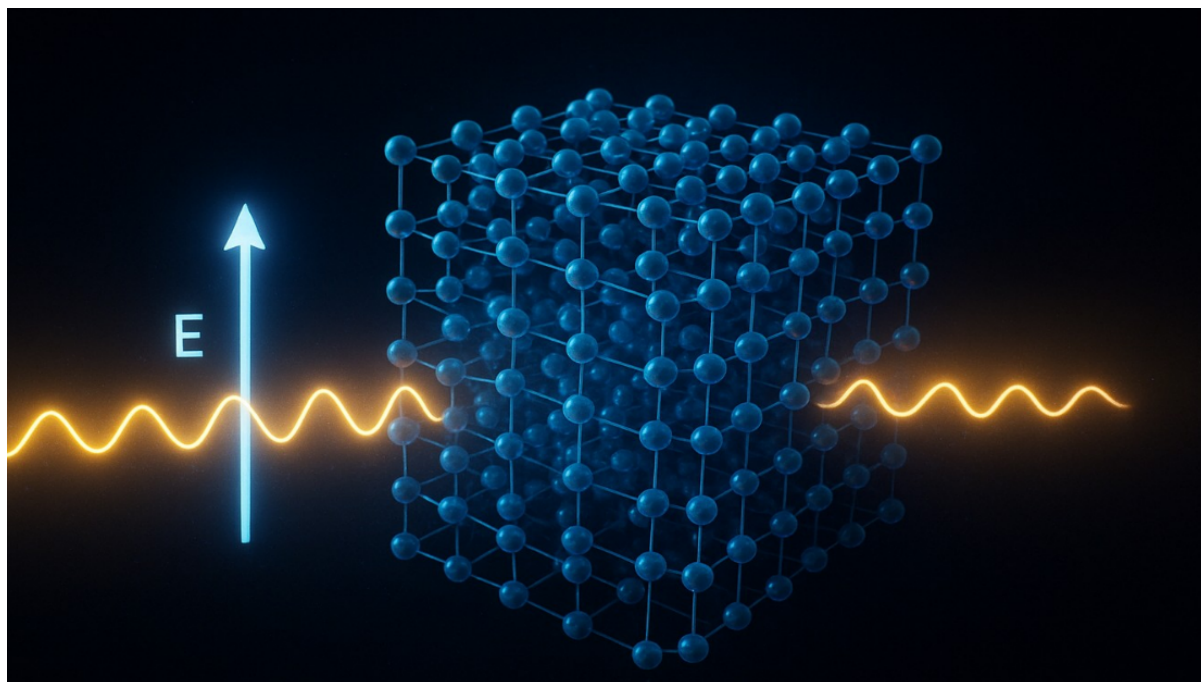


Image by Virginie de Mestral showing the Pockels effect: an incoming laser beam changes phase as it propagates through the crystal under the application of an electric field.