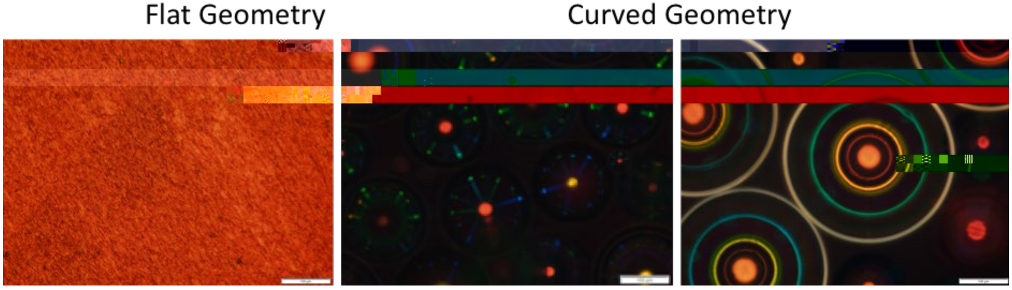
Project 1: Self-organized dual-band-gap materials: regular arrangements of cholesteric liquid crystal spheres

Supervisors: Prof. Jan Lagerwell and Dr. Yong Geng

Description

Cholesteric liquid crystals are very special liquids which, despite their liquid-like fluidity, have a highly regular arrangement of their anisometric molecules, spontaneously adopting a helical organization within the liquid. Because the refractive index depends on the orientation of the molecules, this helical arrangement gives rise to a periodical refractive index modulation. If the pitch of the helix is similar to visible light wavelengths, this self-organization turns cholesteric liquid crystals into optical bandgap materials, that is, light with wavelength equal to the pitch cannot propagate and is instead strongly reflected. Differently to ordinary optical bandgap materials, however, this applies only to circularly polarized light with the same handedness as the cholesteric helix. The reflections are thus not only distinct in color, but they are also circularly polarized. Over the recent years we have studied the optical properties of cholesteric liquid crystals confined in curved geometries—droplets and shells—with the helix axis in the surface normal direction. A variety of intricate colorful patterns arise, very different from the uniform color from cholesterics in flat geometry. In this project we will use cholesteric liquid crystal spheres to build a dual-photonic bandgap material, namely by adding an additional periodicity by periodically arranging the spheres with suitable separations and in relevant geometries. We will study the resulting structures and their optical properties, with the aim to develop advanced multi-functional materials. This is an ambitious project that requires strong dedication by the student. In return, publication in a high-quality international scientific journal is expected.



Microcopy images of selective reflections from cholesteric liquid crystals confined in different geometries.

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Project 3: Assessment of new class of metrics in machine learning models for the prediction of molecular properties

Responsible persons: Valentin Vassilev Galindo / Prof. Alexandre Tkatchenko

Description

Machine learning (ML) is an efficient tool that can provide accurate prediction of molecular properties without the big computational cost of highly accurate *ab-initio* methods [1,2]. Such properties are crucial for successful compound design in chemistry and pharmacy, for instance, for drug discovery, where the molecules should meet specific requirements. Among the available ML approaches, Kernel Ridge Regression (KRR) methods are data efficient and can serve to unveil the underlying laws within the data. However, their success strongly depends on the selection of the distance function inside the kernel, which allows to set the similarities of points in the high-
in order to improve the behaviour of such metrics in high dimensions, trying to avoid the so-
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L^2 norm) have been proposed, showing promising results in learning problems of high-dimensional and structured data. Still, to the best of our knowledge, the use of such metrics in ML for Quantum Chemistry is limited.

Hence, in the present project, we will assess the performance on the prediction of molecular properties using KRR with new type of metrics (fractional, d^p and normalized d^p norms) compared to those normally used (e. g. Manhattan, Euclidean). To accomplish this task, we will employ the QML code [3] and available datasets, like the chemical databases GDB-13 (970 million compounds) and GDB7 (4.2 million structures). For a broader comparison, different descriptors will be used, since the effectiveness of a given metric varies with the
n important knowledge
on how the metric influences the recognition of differences between molecular configurations and how it affects the learning of molecular properties.

Activities

- Review the state-of-the-art machine learning methods for the prediction of physicochemical properties of molecules and the role of metrics in KRR learning.
- Learn how to construct ML models.
- Implementation of the new metrics in the QML code.
- Analysis of the obtained results.
- Writing of the bachelor thesis.

Expected result

Bachelor thesis and a possible peer-reviewed publication.

References

[1] Hansen, K., *et al.*, *J. Chem. Theory Comput.* **9**, 3404-3419 (2013).
[2] Sauceda, H. E., *et al.*, arXiv:1909.08565 (2019).
[3] Christensen, A. S., *et al.*, QML: A Python Toolkit for Quantum Machine Learning (2017).

Project 4: Beyond fermions and bosons in one dimension

Supervisor: Prof. Thomas Schmidt

Description

Physicists are working hard on the unambiguous observation of a new type of particle with behavior that goes beyond the typical description of fermions and bosons, namely the anyon. It is expected that such behavior can emerge when several particles go together to form a quasiparticle under a set of geometric constraints. In this project we will be studying a recent proposal that such anyons can be found in one-dimensional systems when three particles can pass by each other in pairs, but not all at the same time. We will look at some simple models of such a system, and combine cutting edge numerical methods with group theory to study the exotic behavior of an anyon.

Expected result

Bachelor thesis and a possible peer-reviewed publication.