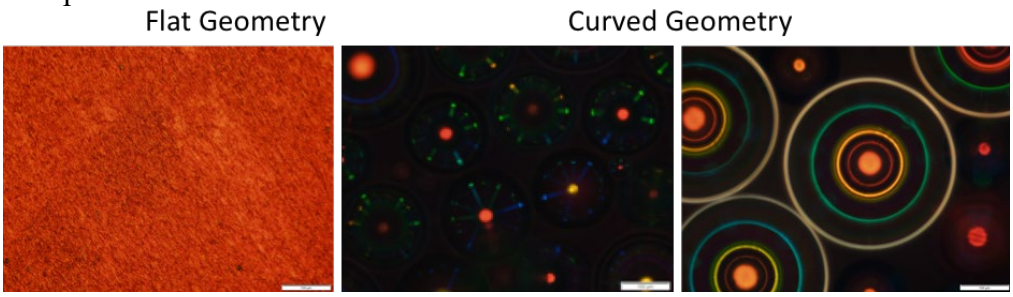
Project 1: Self-organized dual-band-gap materials: regular arrangements of cholesteric liquid crystal spheres

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.

胆甾相液晶珠构筑自组装双带隙材料

胆甾相液晶是一种常见的液晶材料。它是一种特殊的流体，不但具有一般流体的流动性，其分子还具有规则的长范围取向有序，且呈螺旋结构排列。由于材料的宏观折射率取决于分子的平均取向，因此在胆甾相液晶内部折射率空间上呈周期性螺旋结构分布。当光波长与液晶内部螺旋结构的螺距相近时，手性与胆甾相液晶螺旋结构相同的圆偏振光将不能透过，而被部分或者全部的反射，此时胆甾相液晶被称作光子晶体。与普通的光子晶体相比，这种材料的反射光不仅具有取决于其周期结构大小的不同颜色，还有其螺旋结构决定的手性。近年来，本小组研究了受限于曲面结构下的胆甾相

液晶珠以及核壳结构的内部结构以及光学特性，并发现了非同寻常的光学图案。本项目拟通过将胆甾相液晶施加额外周期性限制，从而构建更高级别光子晶体，研究其内部结构和光学特性，研发多功能材料。这是一个有创新，有挑战，同时也是高回报的项目，研究成果有望发表于国际高水平期刊。

Project 2: Machine learning-based model for the prediction of DFTB repulsive potentials

Supervisors: Dr. Leonardo Medrano Sandonas / Prof. Dr. Alexandre Tkatchenko

Description

Machine learning (ML) has been proven to be an extremely valuable tool for the efficient exploration of potential energy surfaces by interpolating coarse data obtained from highly accurate reference methods. For many systems, this allows for simulations with ab-initio accuracy at the computational cost between classical interatomic potentials and density-functional approximations. Similar computational efficiency can only be achieved by semi-empirical methods, such as the density-functional tight-binding (DFTB). However, in contrast to ML-based approaches, DFTB also accounts for quantum-mechanical principles and offers access to a variety of electronic properties by design. Thus, combining these two methodologies opens up a new route for performing faster and accurate calculations of physicochemical properties in a large variety of nanoscale systems.

According to the formulation of DFTB, the repulsive energy in the total DFTB energy mostly contains local interactions and thus represents a very promising target for ML models. Hence, in the present work, we will employ a Neural Network in the form of the SchNet package and the parametrization of the electronic DFTB Hamiltonian will be taken from the 3-ob set of Slater-Koster files. Thanks to the nature of neural networks, our approach requires only minimal user-input and is less subject to a given choice of the descriptor or representation, while allowing us to accurately reproduce DFT energies and forces. This approach will be applied to a database composed of non-equilibrium structures for stereoisomers and conformers of GDB7 molecules, which contains in total about 4.2 million structures. For comparison, we will also perform a study with Kernel method for the prediction of the repulsive energy by using QML code. This work will provide a robust and reliable method for quantum-mechanical simulations of a wide range of systems including non-covalent complexes, which would represent a daunting task for purely ML-based approaches.

Activities

- Review the state-of-the-art of machine learning methods for the prediction of physicochemical properties of molecular systems.
- Learn DFTB method and how to develop ML models with SchNet and QML codes.
- Development of post-processing tools.
- Analysis and discussion of the obtained results.
- Writing the bachelor thesis.

Expected result

Bachelor thesis and a possible peer-reviewed publication.

Exploratory task

Depending on the development of the research work, we could work on the implementation of the DFTB-ML models within the framework of the DFTB+ code.

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-dimensional "feature space". In this regard, many efforts have been made in order to improve the behaviour of such metrics in high dimensions, trying to avoid the so-called "curse of dimensionality". Alternatives to the typical distances (such as the Euclidean-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 description of the data in the "feature space". This work will provide an 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.