2025 Summer Project

Computational Electronic Structure Theory (CEST)

Group leader: Prof. Patrick Rinke

Introduction to the CEST group:

CEST, lead by Prof. Patrick Rinke, is a multidisciplinary research group with expertise in physicists, chemists and machine learning. The CEST group focuses on developing electronic structure and machine learning methods and applies them to pertinent problems in material science, surface science, physics, chemistry and the nano sciences. You can find more informations about CEST on our **website**. For 2025, we are offering two summer research projects for students interested in applying electronic structure theory and machine learning to materials science.

Summer trainees will be an integral part of our team of ambitious and talented researchers. We offer two research projects suitable for both B.Sc. and M.Sc. students:

P1 Modeling and machine learning for plasmonic enhancement of chiral signals

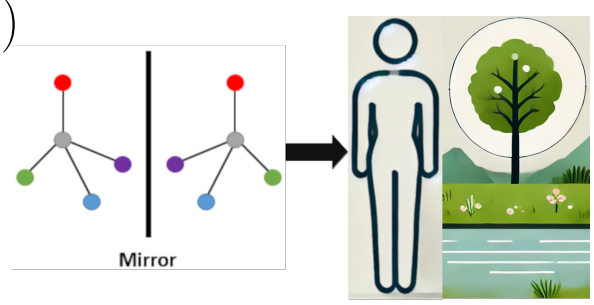
P2 Computational materials exploration and design of perovskite-inspired materials

Submit your application through the *Department of Physics summer trainee application system* and indicate in which research project (1 or 2) you are interested in.

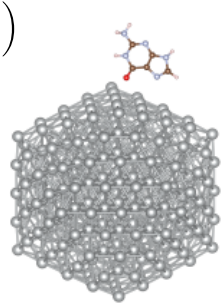
Project 1: Modeling and machine learning for plasmonic enhancement of chiral signals

Project Leaders: Prof. Patrick Rinke and Dr. Maria Weseloh

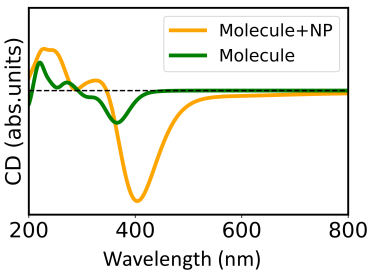
a)



b)



c)



Project description:

Chiral interactions with impact.

A molecule's chirality (handedness) may determines its smell, taste, environmental impact, or effectiveness as medicine (illustrated in panel a). The presence of wrong-handed molecules in drugs can even lead to fatal consequences[a]. Therefore, a reliable detection of molecular chirality is necessary to protect people and the environment. Chirality can be detected in circular dichroism (CD) spectra. However, for many molecules CD signals are below the detection threshold. In this project, we will investigate computationally, if and how plasmonic nanoparticles (NPs) can enhance molecular CD signals (panels b and c).

Join exploring electronic interactions for CD enhancement!

We combine quantum mechanical modeling with machine learning (ML) to characterize plasmonic CD enhancement. Our approach enables, for the first time, the investigation of realistically sized NP-molecule hybrid systems without simple models.

Are you ready for plasmonic CD enhancement?

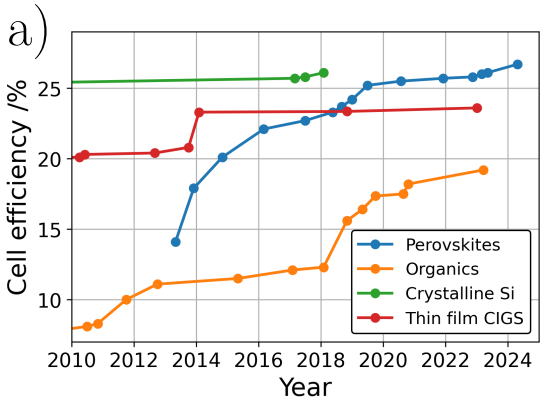
We offer excellent training in quantum mechanical modeling and machine learning. We are seeking a highly motivated student with strong interests in programming (e.g. Python), quantum mechanical modeling, and machine learning to become an integral part of our team.

[a]Tokunaga *et al.*, Sci. Rep. 8,17131 (2018), Ceramella *et al.*, Appl. Sci., 12, 10909 (2022)

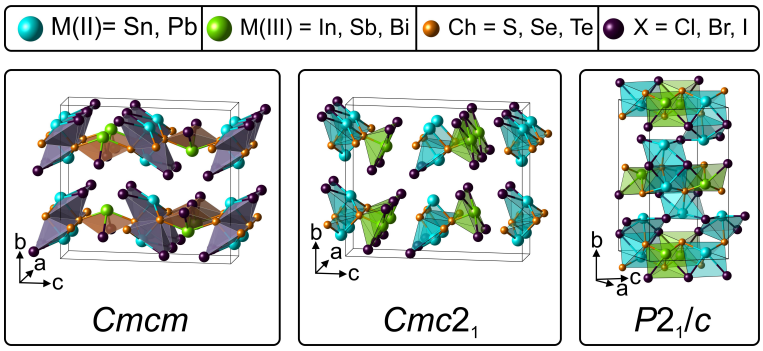
Project 2: Computational materials exploration and design of perovskite-inspired materials

Project Leaders: Prof. Patrick Rinke and Dr. Pascal Henkel

a)



b)



Project description:

Would you like to participate in the solar technology revolution?

Perovskites are the rising stars among the emergent solar-cell technologies and over the last two decades, perovskite solar cells (PSCs) have risen to record efficiency of $\sim 26\,\%$ (panel a). However, commercialization is hampered by toxicity and stability problems. In this context, perovskite-inspired quaternary mixed-metal chalcohalides (MMCHs) with chemical formula $M(II)_2M(III)Ch_2X_3$ (panel b) have the potential to overcome these problems. Furthermore, their crystal structure (panel b) lends itself to element substitution, which could facilitate materials design to the required properties.

Are you interested in cutting-edge computational materials science?

Much remains to be learned about MMCHs due to their novelty. The CEST group has a successful track record in computational modeling of perovskites and MMCHs. In this project, we will use quantum-mechanical (QM) modeling to explore promising lead-free MMCHs materials which have the potential to foster the development of PSCs.

Would you like to apply QM modeling and machine learning in practice?

QM modeling can provide reliable data for machine learning (ML), which can then accelerate materials discovery. Through the combination of QM and ML, interesting perovskite-inspired MMCHs can be investigated efficiently and reliably in order to answer scientific questions. We hope you are interested and motivated to learn more about QM modeling (density functional theory), ML and programming (e.g. Python) while diving into materials science over the summer as an integral part of our team.