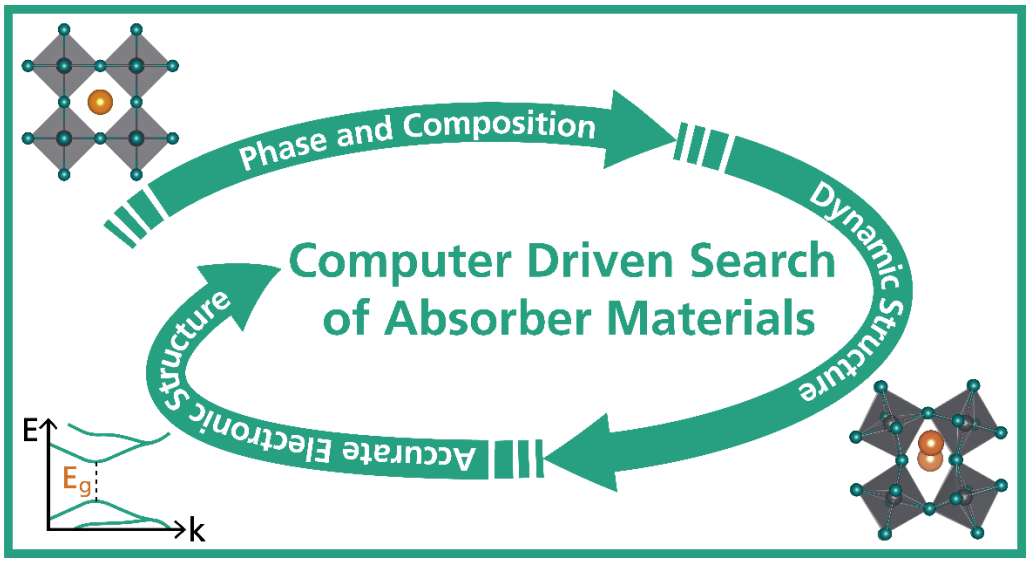

Master Thesis Project:

Quantum Mechanical Calculations of Absorber Materials for Lead-free Solar Cells at Device Operating Conditions

In this project, you will learn how to use computational methods of electronic-structure theory to study the light harvesting behavior of next generation solar cells under device operating conditions. You will apply theoretical models to practical applications.

Mixed organic-inorganic perovskite halides have emerged as most promising absorber materials for the next generation of solar cells. These soft materials have highly dynamical structures at device operating conditions, which lead to drastic changes of the optoelectronic properties. Thus, materials modeling must take these effects into account to explain experimental findings and to drive materials development. With a recently developed computational workflow, this difficult task is now efficiently doable. We want to employ this methodology to study tin- and germanium-based perovskites at device operating temperatures. These materials have the potential to substitute lead-containing perovskites, which currently achieve best solar-cell efficiency but are critical for the environment.

In this master thesis project you will learn:

- how to do state-of-the art density-functional theory (DFT) calculations, supplemented with corrections that mimic the complex many-body behavior of the electronic system
- how to run ab initio molecular dynamics simulations and how to evaluate the effect of structural dynamics on optoelectronic properties
- to investigate perovskites containing Sn and Ge instead of Pb as potential candidates for next generation solar cells

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Further Reading: Gebhardt, J., Wei, W., & Elsässer, C. (2021). Efficient Modeling Workflow for Accurate Electronic Structures of Hybrid Perovskites. *The Journal of Physical Chemistry C*, *125*(34), 18597–18603.