Quantum mechanical exploration of solar technologies
2016 Summer Project

Project description

Would you like to research a novel material in the photovoltaic revolution?
Hybrid perovskites are a novel materials class that is currently shaking up the solar cell world. Current solar-cell technologies are based on inorganic materials, such as silicon, that tend to be expensive. In hybrid perovskite photovoltaics (HPPVs) organic molecules are intermixed with a trihalide perovskite (right Figure) that is cheap to produce and promises affordable energy from the sun. HPPVs rose to record efficiencies (~20%) in only four years after their discovery (left Figure).

Do you enjoy quantum mechanics and computer simulations?
Due to their novelty, much is still to learn about hybrid perovskites. In this project we will investigate hybrid perovskites on the most fundamental level: quantum mechanics. Using simple models and computer simulations we will study the atomic and electronic structure of hybrid perovskites and the light-to-energy conversion process. The objective is to develop a quantum mechanical understanding of these novel materials that leads to a further increase in the solar cell efficiency or device longevity.

Computational Electronic Structure Theory (CEST) group
Project leaders: Prof. Patrick Rinke, Dr. Hugo Levard and Dr. Jingrui Li