# Theoretical Methods in Spectroscopy

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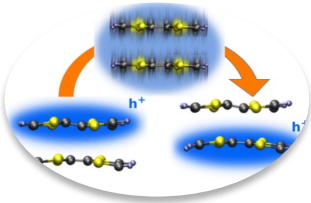
## Simulation of Electronic Processes

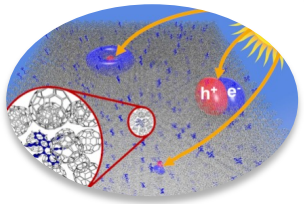
The major goal of our research is the development and application of highly efficient **theoretical and computational methods** to describe physical properties of chemical compounds in various application fields. This ranges from electronic properties and charge transport to optical, thermoelectric or photovoltaic properties.

Controlling electronic processes is a great challenge because of interesting effects from the quantum world and interesting materials with each material having its own specific set of properties. This makes predictions and simulations a great endeavor, where theoretical modelling is often closely linked to experiments or material design.

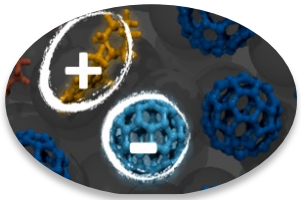
For instance, in the field of *covalent organic frameworks*, we aim at predicting novel 2D COF structures based on molecular and supra-molecular simulations. The simulations "*from molecules to functions*" span multiple length and time scales.




Charge Transfer and Transport

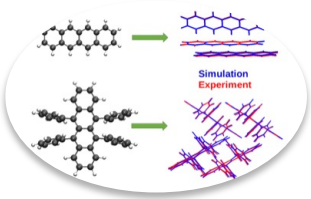



Organic Solar Cells

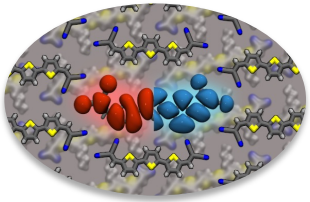


Semiconductor Doping

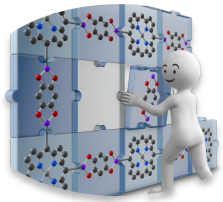
Computational Methods




Crystal Structure Prediction



Band Structure Engineering



2D Covalent Organic Frameworks