

## Research Project

### 3-Dimensional Molecular Acceptors for Efficient Electron Transport Materials

#### Third-party funded project

**Project title** 3-Dimensional Molecular Acceptors for Efficient Electron Transport Materials

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**Organisation / Research unit**

Departement Chemie

**Department**

**Project start** 01.09.2017

**Probable end** 31.08.2021

**Status** Completed

The estimates for the energy consumption growth forecast its increase by more than 50% by 2040, in particular due to high demand for energy in rapidly growing economies of the developing countries. The global warming threats leave us no choice but to rely on the production of clean energy, where the solar energy will slowly become our most important source to produce electricity due to its abundance from the sun. The production of electricity must, however, be as cheap as possible to compete with the well-established production of electricity from fossil fuels, such as coal and natural gas. This requires implementation of inexpensive and environmentally friendly materials into solar cells. In this regard, organic materials offer the solution because they can be produced cheaply on a large scale. The problem with organic photovoltaic devices is, however, their low power conversion efficiency, which is a consequence of the short exciton-diffusion lengths and imbalanced charge transport in organic materials with lower mobility of electrons than that of holes. Simultaneously, the best performing electron-transporting materials in organic solar cells, namely, fullerenes, absorb visible light poorly, are hard to modify, and expensive to produce. In this research proposal, the synthesis and experimental investigation of shape-persistent macrocycles, covalent organic cages, and nanotubes with built-in molecular electron acceptors is described. The symmetric spatial arrangement of these molecules, and the control of the mutual distance and orientation of the acceptor units will allow to study the charge photogeneration and the subsequent transport of electrons in the materials incorporating them as a function of relatively few structural parameters. The unique shape of the proposed macrocycles will, in addition, allow to grow highly crystalline materials for charge transport in solution or on surfaces. In combination with the facile synthesis, tunable light absorption, electronic, and solid-state properties of these molecules, the macrocycles, cages, and nanotubes will, one day, allow for substituting the fullerenes to make efficient organic solar cells commercially available and competitive with other photovoltaic technologies.

**Keywords** time-resolved spectroscopy; molecular cages and molecular nanotubes; organic thin films; electron paramagnetic resonance spectroscopy; organic photovoltaic devices; covalent organic frameworks; organic synthesis; electron transport; crystal growth

**Financed by**

Swiss National Science Foundation (SNSF)

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