

Perovskites for Solar Energy

Overview

Introduction

Hybrid perovskites solar cells are a promising solution in the field of photovoltaic devices to overcome the efficiencies/cost ratio of conventional solar cells. The understanding of the processes upon absorption of light in these materials will aid to a rational improvement of their performances.

Objectives

We aim at establishing an iterative strategy in order to improve the efficiencies of perovskite solar cells going from the synthesis and preparation to spectroscopic studies of the charge carrier dynamics and their theoretical simulations. Each study will feed back into the others aiming to a rational improvement of the device performance.

Perovskite thin film solar cells

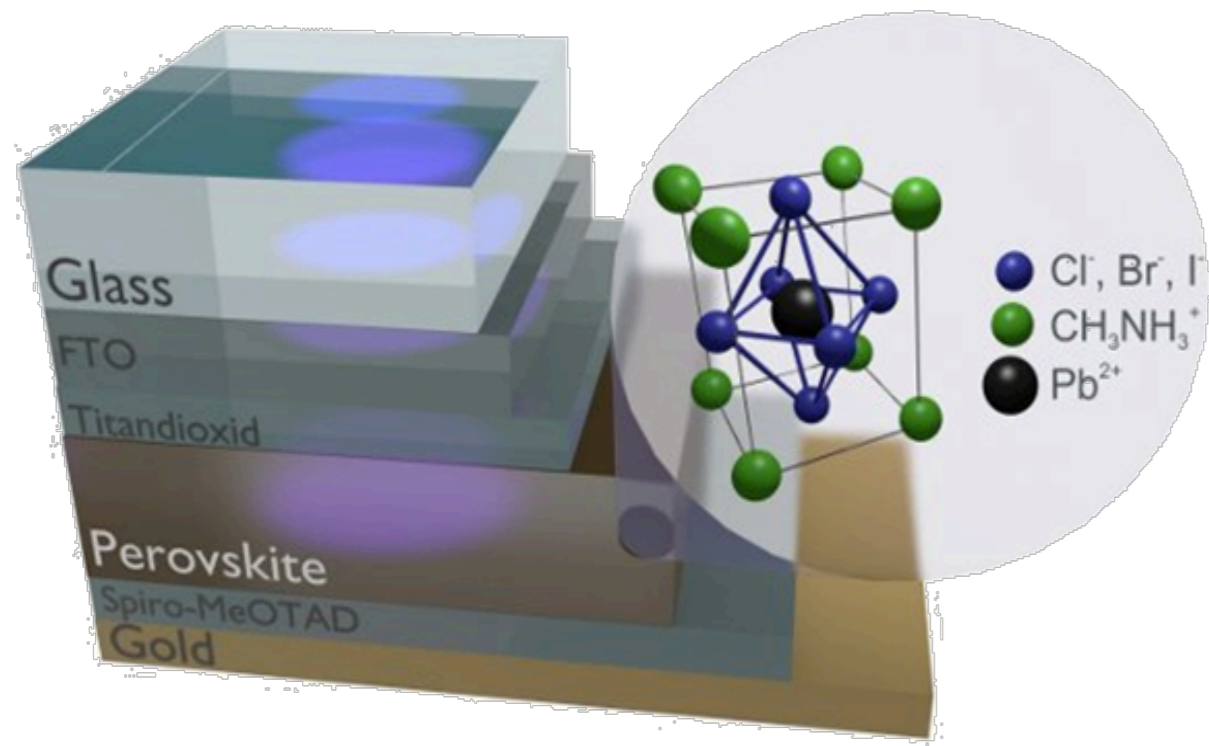


Fig. 1 – Schematic perovskite solar cell structure

Figure 1 shows a typical perovskite-based solar cell architecture. We will use three different preparation methods (Fig.2):

- (a) One-Step Precursor Deposition (OSPD);
- (b) Sequential Deposition Method (SDM);
- (c) Dual-Source Vapor Deposition (DSVD).

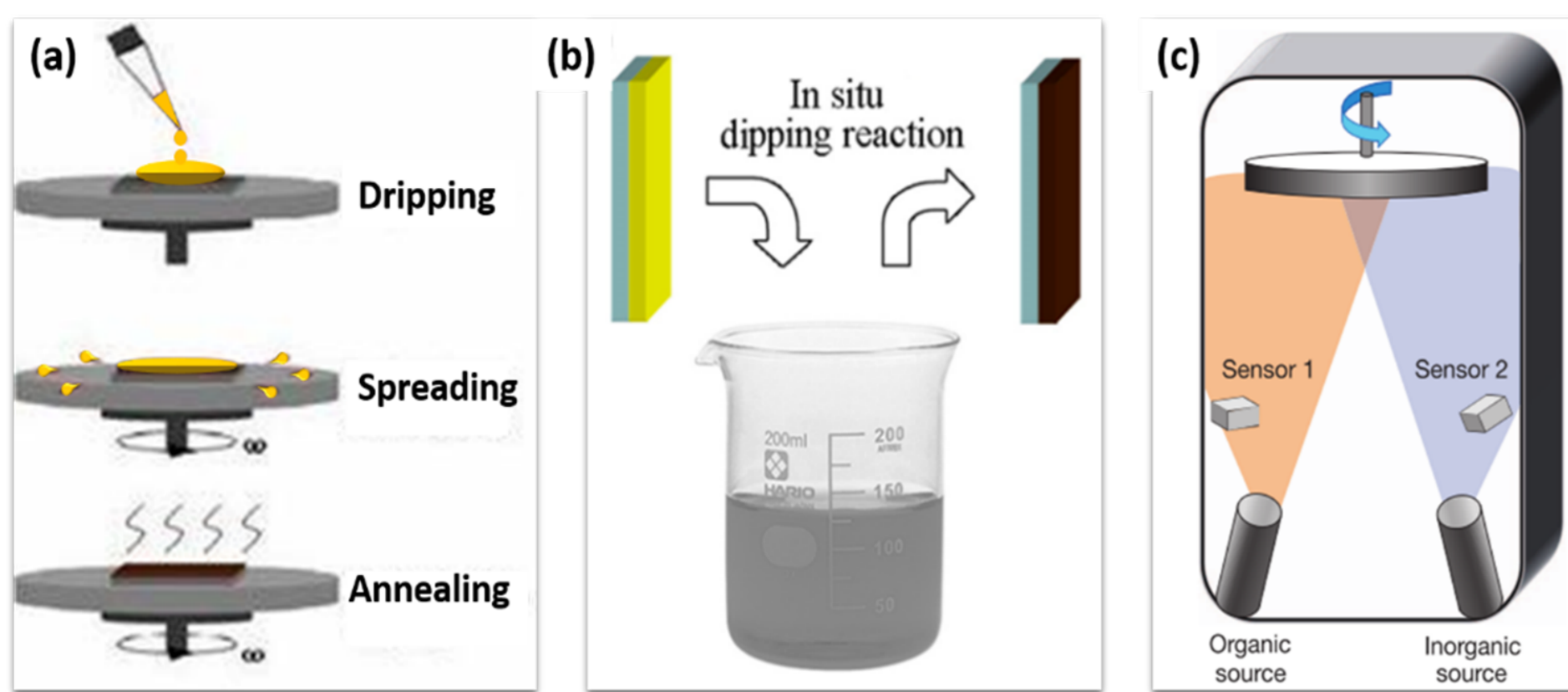


Fig. 2 – Popular perovskite solar cell fabrication methods

Ultrafast spectroscopy

Ultrafast spectroscopy is a powerful tool to investigate charge carrier dynamics, like evolution of excitons, radiative recombination and charge trapping (Fig. 3).

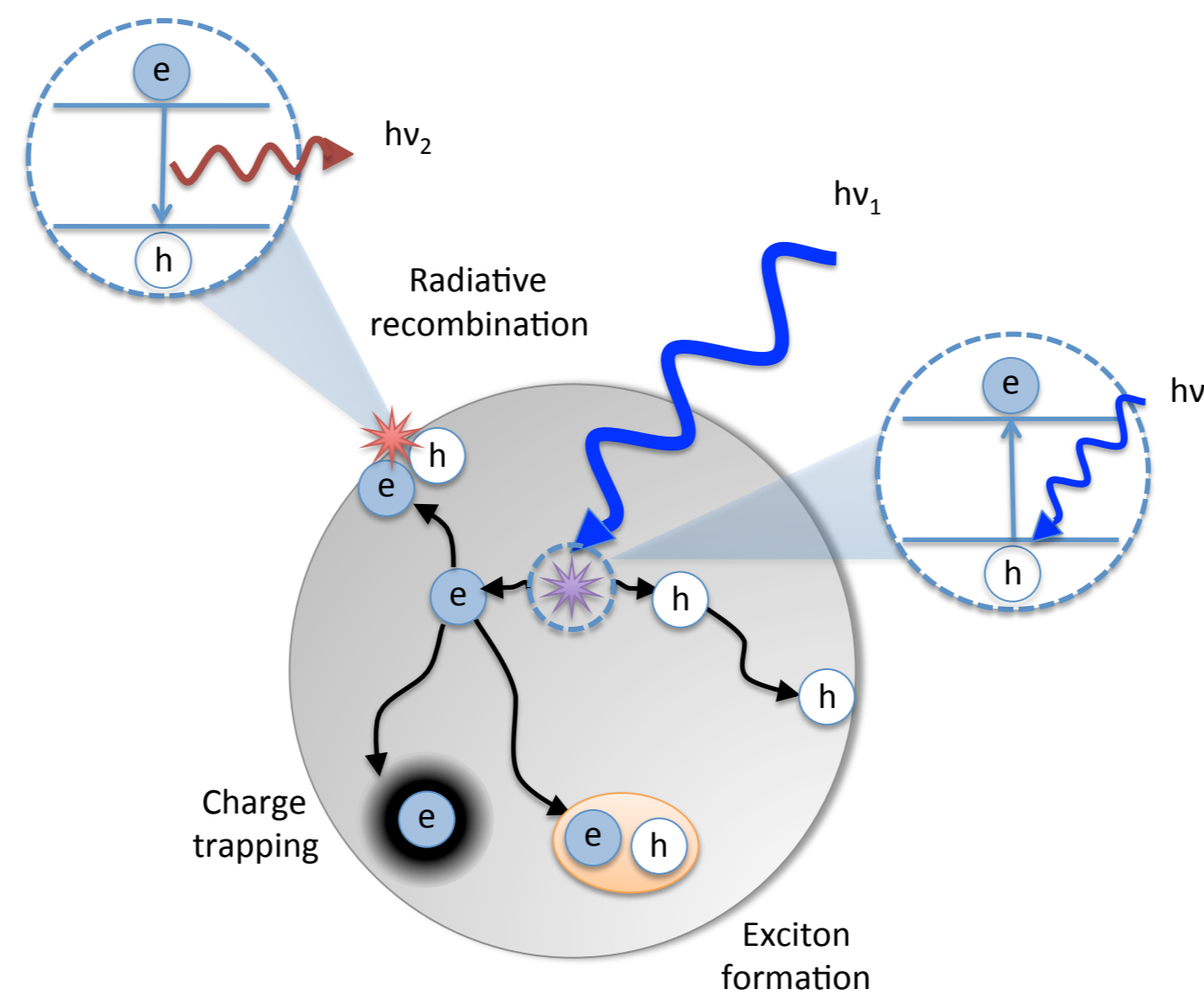


Fig. 3 – Schematic view of ultrafast processes upon light absorption in a perovskite nanoparticle.

We will use: a) transient absorption, b) ultrafast photoluminescence, c) time resolved X-ray absorption, aimed at gaining a deeper insight into the physical processes behind the extraordinary efficiency of perovskite solar cells.

Computational studies

Electronic structure of perovskites is investigated by: a) Density Functional Theory (DFT, Fig. 4), taking into account a) spin-orbit coupling effects; b) GW methods for studying many body effects; c) high-throughput *ab initio* calculations on perovskites differing in cations, halogens and different structural symmetry to study band gap energies and effective masses.

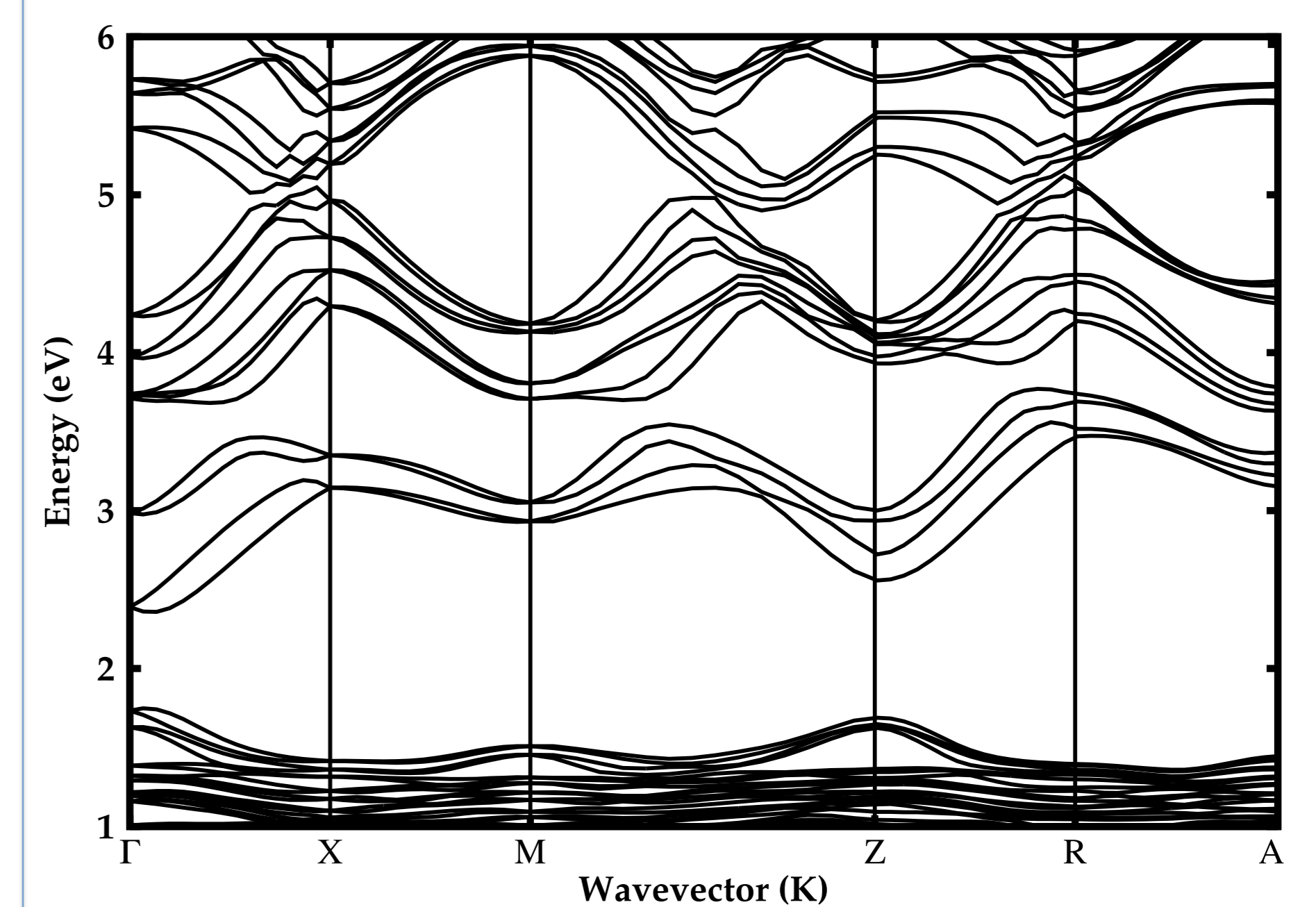


Fig. 4 –Band structure of CH₃NH₃PbI₃

Partners and Collaboration

WP1

Prof. M. K. Nazeeruddin, Dr. P. Gao, Dr. I. Dar
Laboratory of Photonic Interfaces, EPFL

WP2

Prof. M. Chergui, T. Palmieri, F. Santomauro
Laboratory of Ultrafast Spectroscopy, EPFL

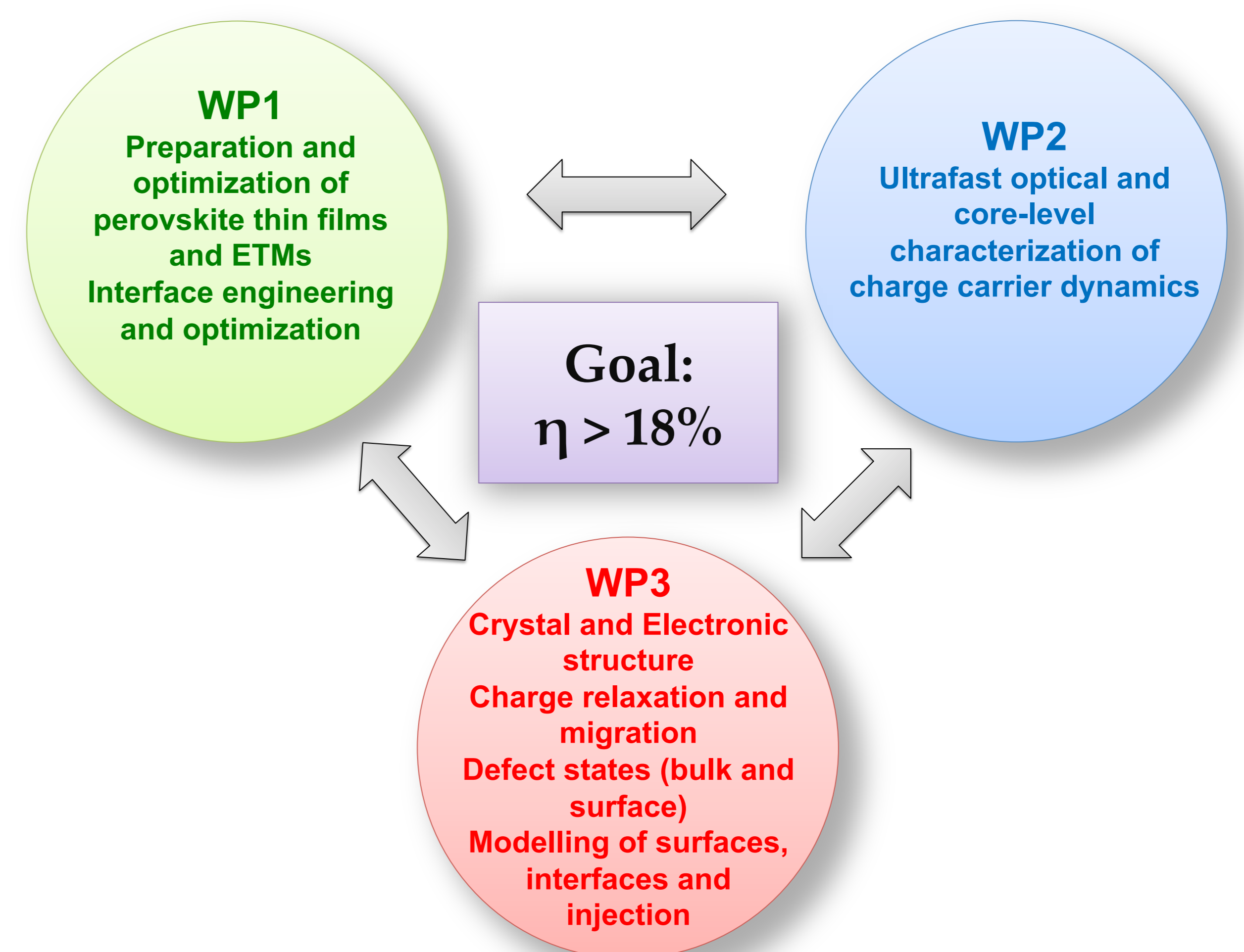
WP3

Prof. U. Röthlisberger, A. Boziki, N. Ashari Astani
Laboratory of Computational Chemistry and Biochemistry, EPFL

Collaborations:

- Synthesis of CsPbX₃ nanocrystals
- Prof. M. Kovalenko, Functional Inorganic Materials, ETH
- Synthesis of thin films
- Prof. A. Hagfeldt, Laboratory of Photomolecular Sciences, EPFL

Energy Turnaround



Contact

Prof. M. Chergui, Laboratory of Ultrafast Spectroscopy, EPFL - majed.chergui@epfl.ch

Prof. M. K. Nazeeruddin, Laboratory of Photonic Interfaces, EPFL - mdkhaja.nazeeruddin@epfl.ch

Prof. U. Röthlisberger, Laboratory of Computational Chemistry and Biochemistry, EPFL - ursula.roethlisberger@epfl.ch