Numerical simulation of optoelectronic devices based on perovskite materials

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FOTON-OHM laboratory has developed an expertise in simulation, design, growth and characterization of semiconductor nanostructures for photonics applications. Research is dedicated to telecommunication applications on InP substrate as well as more recently to silicon photonics (ongoing ANR projects) including light emitters, photodetectors and solar cells. In the photovoltaic (PV) field, Hybrid organic-inorganic perovskites (HOP) have recently entered the competition for new PV materials with unprecedented speed and impact. In less than five years HOP thin film prototype cells have more than quadrupled their efficiency, and produced electrical power, to reach over 23% in single junction in 2018, and over 26% in solar cell tandems. Perovskite solar cells are now leading both thin film and quantum dot–based solar cell technologies. Their efficiency also exceeds typical values for commercial Si cells and comes close to the best Si-based crystalline solar cells. However a deep understanding of the physical properties of these unconventional hybrid semiconductors is still lacking in order to optimize the process parameters as well as the devices structures. Hence, many important issues like hysteresis, bulk and surface carrier recombination effects have still to be addressed.

In the field of hybrid perovskite cells, FOTON has an international leading position, and the simulation group shares his activity in three strongly correlated fields: the theoretical study of materials and nanostructures optoelectronic properties (using state of the art of ab-initio or empirical methods), the collaboration with experimental groups on spectroscopy and structural properties of perovskite materials and devices, and the multi-scale numerical device simulation.

The proposed PhD thesis aims at using the state of the art industry-based Silvaco numerical code to simulate perovskite based optoelectronic devices: Solar cells, Light-emitting diodes (LED) and Thin Film Field Effect Transistors (TFT). The application of the solar cells is now enlarged by FOTON laboratory to the multi-junctions (tandems …) structures for low-cost and high performance single junction solar cells, in collaborations with state of the art experimental groups. The study of the later device can bring further understanding of the hysteresis effect attributed to ion migration in the perovskite layer, as well as progress to enhance solar cell stability under light soaking. This work will be done in close collaboration with the technology and characterization teams of French and foreign partners laboratories in order to assess the physical parameters used to describe the microscopic and macroscopic properties of the materials and the device structure.

References on perovskite device simulations:

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References on experimental studies of perovskite materials and device:

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