

\* or Specialisation

\*\* Physics or AFM

## Bachelor\*- or Master\*\* Thesis Projects

### Simulation of organic solar cells with machine learning

#### Motivation

Solar cells represent a very important contribution to the energy mix of the future. They are inexpensive and can be manufactured by means of efficient production using printing machines, and are operated CO<sub>2</sub>-neutral.

In the tendered work, organic solar cells are to be simulated with the program [gpvdm](#) by Prof. Roderick MacKenzie, so that our experimental findings are reproduced correctly.

#### Tasks

The offered bachelor and master theses have in common that they deal with the simulation of modern organic solar cells - which have efficiencies in the range of 13% - 16% - in order to better understand these components.

We offer variously oriented topics:

1. What charge carrier mobility is measured in the Time Delayed Collection Field experiment? Background: the experiment is based on the time-dependent extraction of charges, but electrons and holes cannot be distinguished directly. Is the faster type of charge carrier measured, or the average value, or the slower?
2. The physical parameters of organic solar cells will be determined using data from complementary experiments in our group. This will be done either by global fits, which are already implemented in gpvdm, or by deep machine learning, as already shown by Roderick MacKenzie and us on model systems (see above right). Background: the parameters allow a better understanding of the physical processes in the solar cell. Up to now, however, simulated and measured current-voltage characteristics have been used for the fits. In the future, the parameter determination will be deepened and improved by including complementary measurement results, e.g. impedance spectroscopy and light-modulated photovoltage measurements.

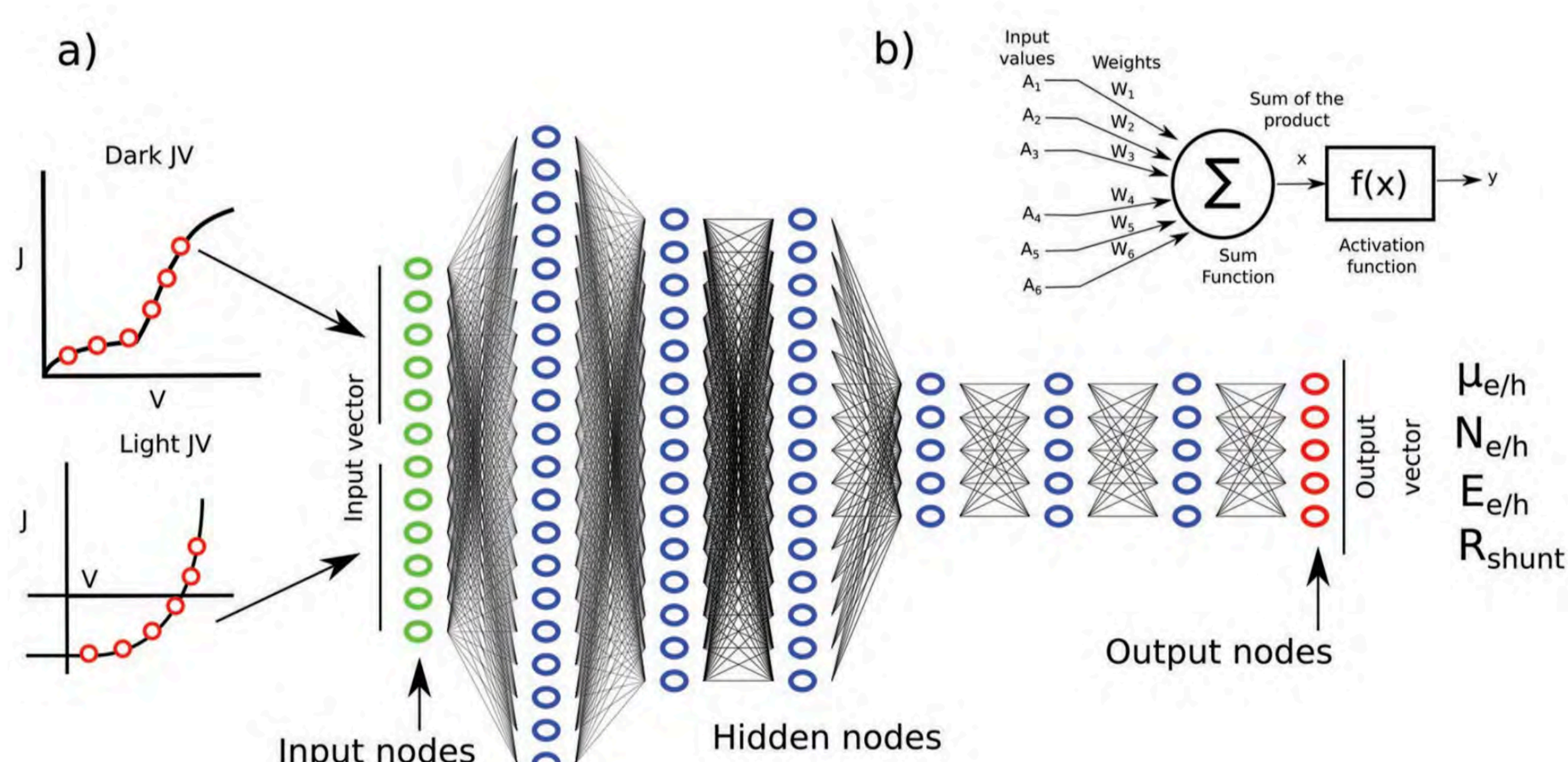
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#### Using Deep Machine Learning to Understand the Physical Performance Bottlenecks in Novel Thin-Film Solar Cells

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Scheme of the neural network, which is trained with simulated data and serves to determine the physical solar cell parameters.

#### Prerequisites and Supervision

You should be interested in theoretical work on the physics of organic solar cells, with a powerful simulation program as a tool. The exact occupation with technical literature is part of the work as well as the discussion of the results within our group in English language. **This interesting work is jointly supervised by Prof. Deibel and Prof. MacKenzie.** If you are interested, you can also produce your own solar cells and conduct experiments. **Under the current conditions it is in principle possible to carry out the work from the home office;** a close connection with various means of communication (email, video conference, etc.) is offered and its use is expected.