Available PostDoc position (1+1 years)

Prof. Alessio Gagliardi, "Simulaton of Nanosystems for Energy Conversion"

**WHAT:** development of a new simulation platform for high-throughput screening and *in-silico* synthesis of new organic semiconductors (small molecules and polymers) with top electrical and optical properties for field effect transistors and solar cells. Towards a fast rational design of organic semiconductors.

**WHY:** Despite the huge development of organic semiconductors (OS), there are still many aspects of these materials underdeveloped and new paths that need to be exploited. An indication of this are the recent breakthroughs regarding blended materials for high mobility solution processed films and copolymering for tuning the light absorption/emission spectrum. One of the main reason of this slower progress is the approach to OS research still largely based on a trial-and-error method. This fact, joint to the huge number of possible materials that can be synthesized, makes the exploration of novel solutions a time and cost consuming business which has reduced the technological transfer of these materials into industry. On top of this, many crucial properties required for performing materials, such as charge mobility, present complex challenges as they are linked not only to the molecular structure but also to the film morphology. This makes *in silico* approaches very time consuming. It is thus mandatory to speed up the development of OS by switching to a more rational design based on modeling, but at the same time strongly reducing the computational cost.

**HOW:** Several *in silico* strategies to switch to a rational design for OS have been proposed. They are based on multiscale approaches where the different spatial scales of electrical and optical properties are addressed in a hierarchical multiscale numerical model. However, such methods are tremendously computational expensive. The project goal is a Multiscale-Multiphysics-Machine (Deep) Learning (ML/DL) approach where Multiscale models are merged with state-of-the-art Machine(Deep) Learning algorithms to speed up the calculation. This reduces significantly the computational cost (up to 100 times faster).

The project is a purely theoretical work at Prof. Alessio Gagliardi’s group (Technical University Munich).

**Specific tasks:**

1. Develop new machine (deep) learning approaches to speed up multiscale simulations for OS electrical and optical properties;

2. Use of different numerical models: atomistic density functional theory, molecular dynamics, kinetic Monte Carlo.

3. Excellent programming skills (C++, Object Oriented Programming)

4. Supervising PhD students and Master students;

5. Teaching skills;

**Starting date:** soon in the next few months

**Salary:** 100% TV-L E 13 position for 24 months (1 year contract, extendable to another year: 1 + 1)

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