INKA: Inks for large-scale processing of polymer solar cells

The DTU-based researchers of the NOMAD consortium, led by the NOMAD Pi Kristian Thygesen, are involved in the INKA project which aims to push the commercialization of polymer solar cells (PSC). They will do so by addressing the crucial bottleneck for their industrial manufacture: the highly limited access to robust, cost-effective inks for the processing of the photoactive layer of the PCS.

The INKA project is sponsored by the Danish Innovation Fund as a collaboration between DTU, the Danish companies Grafisk Maskinfabrik A/S -a supplier of machines for PSC processing-, and the start-up company infinityPV ApS, who supplies solar cells, inks, materials and services for PSC processing. To project covers all the important aspects of R&D based PSC production, from first-principles modeling of novel light-absorbing polymers, to chemical synthesis and processing of inks, to demonstration and testing of the inks in an industrial environment.

In the context of the NOMAD CoE, DTU is performing an extensive computational screening of the organic donor-acceptor molecules that form the basis of the light absorbing conjugated polymers of the PSC. In particular, first-principles calculations of the structure and energy levels of more than 10.000 molecules have been completed at this point and more will follow. This by itself provides a unique library useful for the exploration and identification of polymers with optimal energy levels. In Refs. [1] and [2] below a similar approach was used to identify light-harvesting porphyrin-based molecules for dye-sensitized solar cells.

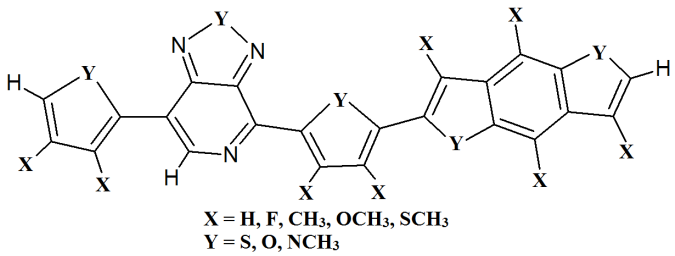

Figure 1: Example of a donor-acceptor monomer from the INKA project. Apart from varying the donor-acceptor backbone, the molecule can be functionalized by different side groups marked by X and Y. Using computational screening the structure and energy levels of a large number (>10.000) of monomers are investigated.

However, even larger opportunities exist beyond the set of calculated polymers: by training the machine learning algorithms developed by the NOMAD team on the established data set, it will be possible to predict the molecular and electronic structure of a much larger space of molecules without new performing new (quantum) calculations and to identify general trends and correlations in the data which in turn can be used to identify novel candidate polymers.

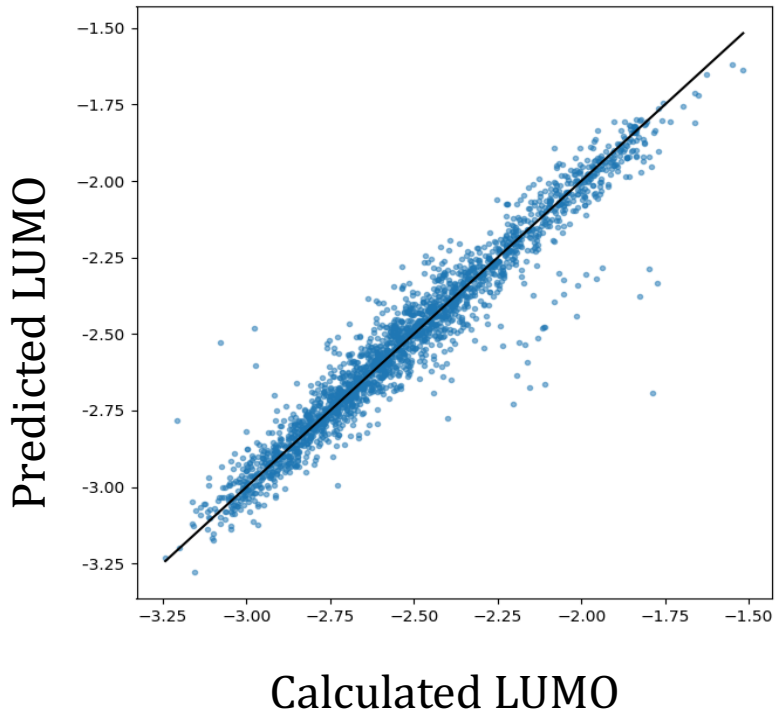

Figure 2: Predicted vs. Calculated (DFT) LUMO levels for the molecule in Fig 1. Training machine learning algorithms on this dataset will enable discovery of new polymers with optimally aligned energy levels for organic solar cells.

[1] **Design of two-photon molecular tandem architectures for solar cells by ab initio theory**, K. B. Ornso, J.M.Garcia-Lastra, G. De La Torre, F.J.Himpsel, and K.S.Thygesen Chem. Science 6, 3018 (2015)

[2] **Optimizing porphyrins for dye sensitized solar cells using large-scale ab initio calculations**, K. B. Oernsoe, C. S. Pedersen, J. M. Garcia-Lastra and K. S. Thygesen Phys. Chem. Chem. Phys. 16,16246 (2014)