Contribution ID: **20** Type: **Poster**

Optimization of thin films in organic diodes using computer simulation

Tuesday, 16 September 2025 16:02 (1 minute)

Computer simulations were carried out to understand the processes that occur in organic light-emitting diode (OLED) devices at an atomic and macroscopic level. The main goal was to optimize the OLED structure by taking into account the transport of charge carriers, quantum efficiency and stability. The characteristics and morphology of subsequent layers and interlayer junctions were also examined, as was the exact relationship between the degree of layer interpenetration and the energy barrier for charge carriers, and the interaction between host-guest complexes in the emissive layer and charge transport properties. To overcome the difficulties associated with the different sizes and timescales of polymer systems, we propose developing efficient coarse-grained computer simulation methods. Simplifying macromolecular systems due to their complexity enables the study of morphology and the electroluminescence effect of large systems over sufficiently long timescales. We used the Dynamic Lattice Liquid model, a variant of the Monte Carlo method based on the concept of cooperative motion. The most demanding cases were performed on the ARUZ dedicated machine in the BioNanoPark in Łódź. A machine learning approach, most likely a neural network, was designed and trained on this data to predict promising combinations of experimental parameters and conditions. This enabled the simulation of phenomena occurring simultaneously for all molecules, significantly accelerating the calculations and enabling the study of systems consisting of millions of elements, as in real OLED layers.

Primary author: SIKORSKI, Andrzej (Faculty of Chemistry, University of Warsaw)

Co-author: Prof. POLANOWSKI, Piotr (Department of Molecular Physics, Łódź University of Technology)

Presenter: SIKORSKI, Andrzej (Faculty of Chemistry, University of Warsaw)

Session Classification: Coffee and Poster Session