TRIPHENYLAMINE-BASED MONOLAYERS FOR OPTOELECTRONIC DEVICES

Aida Drevilkauskaitė[1], Artiom Magomedov[1], Vytautas Getautis[1]

[1]Kaunas University of Technology
aida.drevilkauskaite@ktu.edu

As energy consumption continues to grow, the need for more energy increases. Renewable energy has gained significant interest from both scientists and the industry over the past decade, with solar energy remaining the most popular source. To enhance absorption and efficiency, new technologies need to be developed as well as new materials need to be used.

Even though there is no perfect material for all, self-assembled monolayers (SAMs) are becoming the reference for hole-transporting materials in inverted perovskite solar cells (iPSCs) due to low material cost and simple layer formation. One of the most well-known SAMs is phosphonic acid with a carbazole moiety and different functional groups [1]. Although SAMs have shown promising results, there is still a lack of information on how the molecular structure of the SAMs is related to the electrical properties of the iPSC. Understanding how structural changes in SAM molecules are linked to performance in photovoltaic devices is crucial for modeling molecules with optimal performance and efficiency in different devices.

Phosphonic acid is known to make a strong bond with oxide surfaces [2] Yet, some authors shows that boronic acids might be better option because they are less acidic and potentially more stable in the device [3]. However, boronic acid compounds are known as materials that has lower stability and weaker bond with the surface compared to phosphonic acid. This research aims to determine whether triphenylamine-based phosphonic acid monolayers with different functional groups are a better choice than boronic acids for making efficient and stable solar cells. We used DFT calculations to predict dipole moments. Moreover, materials synthesis was performed using Hirao-Coupling reaction mechanism. The structural characterization was performed using NMR $_{1}$H and $_{13}$C spectra and mass spectrometry. Additionally, devices with the mentioned materials will be constructed and characterized using a solar simulator.

[1] Al-Ashouri, A. et al., Science 2020, 370, 1300–1309 DOI: 10.1126/science.abd40
[2] Paniagua, S.A. et al., Chemical Reviews 2016, 116, 7117–7158 DOI: 10.1021/acs.chemrev.6b00061
[3] H. Guo et al, National Science Review 2023, DOI: 10.1093/nsr/nwad057