SYNTHESIS AND INVESTIGATION OF THE CARBAZOLE BASED PHOSPHONIC ACIDS WITH DIFFERENT ALIPHATIC LINKERS

Aida Drevilkauskaitė, Artiom Magomedov, Ernestas Kasparavičius, Tadas Malinauskas, Vytautas Getautis

Department of Organic Chemistry, Kaunas University of Technology, Lithuania
aida.drevilkauskaite@ktu.edu

Over the last decade, perovskite solar cells (PSCs) have attracted major interest from scientists and industry. It can be attributed to the simple fabrication process and low consumption of materials. In particular, the formation of the functional layers can be achieved without the use of high temperatures via solution processes. To maximize the performance of the final device, it is very important to optimize every individual layer. For example, hole transporting material (HTM) needs to ensure high selectivity to the holes, while simultaneously passivating interface with a perovskite absorber layer.

To ensure a successful transition to the market, apart from efficiency and price, another important parameter is the stability of the devices. In recent work, HTM layer is often described as the weakest link of the PSC, due to the extensive use of the dopants [1]. Therefore, it is important to look for an alternative, dopant-free HTMs, that does not require the use of the dopants.

Recently, as an alternative to the traditional HTMs, hole-selective monolayers were introduced into PSCs with the p-i-n configuration [2]. In this case, instead of a spin-coating, a simple and scalable dipping method can be used. This alternative method is giving several important advantages, i.e. low material consumption, ability to form a layer on the rough surfaces, minimal parasitic absorption, etc. The highest efficiency of 20.8% was achieved with carbazole based phosphonic acid, called 2PACz (Fig. 1. n=2). In this material, carbazole moiety is ensuring high selectivity for holes, while phosphonic acid anchoring group is providing good binding with indium tin oxide surface. Seeing a high potential of monolayer HTMs, further structure optimization was performed.

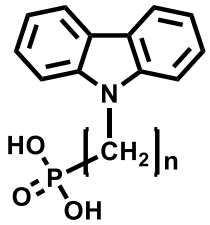

Fig. 1. The general structure of the **nPACz** materials, where n=2, 3, 4, 5, 6.

In this work, a series of new carbazole based phosphonic acids with different aliphatic chain linkers were synthesized (Fig. 1.) It is expected, that longer aliphatic chains could improve the ordering of the monolayer film, however, at the cost of reduced ability to transport charges. To achieve that, the carbazole starting material was alkylated with dibromoalkanes to give intermediate compounds with an aliphatic bromide functional group. In the following step, it was transformed into phosphonic acid ethyl ester, by means of Arbuzov reaction. Finally, ester cleavage was performed using reaction with bromotrimethylsilane, with the subsequent hydrolysis, to give a final compounds **nPACz**. The structures of the synthesized materials were confirmed by ^{1}H and ^{13}C NMR spectroscopy. In future research, the synthesized materials are planned to be tested in photovoltaic devices.

[1] A.K. Jena, A. Kulkarni, T. Miyasaka Halide Perovskite Photovoltaics: Background, Status, and Future Prospects. Chemical Reviews, ACS 119(5), 3036–3103 (2019)

[2] A. Al-Ashouri, A. Magomedov, M. Roß, et al. Conformal monolayer contacts with lossless interfaces for perovskite single junction and monolithic tandem solar cells. Energy & Environmental Science, 12(11), 3356–3369. (2019)