Proceedings of the 3rd World Congress on Recent Advances in Nanotechnology (RAN'18)
Budapest, Hungary – April 10 - 12, 2018
Paper No. ICNNFC 146
DOI: 10.11159/icnnfc18.146

Efficient Chemometric Approach Supporting the Design of Fullerene Derivatives for Solar Cells

Celina Sikorska
Department of Theoretical Chemistry, Faculty of Chemistry, University of Gdansk
Wita Stwosza 63, Gdansk, Poland
celina.sikorska@ug.edu.pl

Extended Abstract

Remarkable physicochemical features of fullerene derivatives (FDs, such as [6,6]-phenyl-C_{61}-butyric acid methyl ester (PCBM) or [6,6]-thienyl-C_{61}-buteric acid methyl ester (TCBM)) offer a great potential in applications of biological chemistry and in the materials science and thus have been a major topic in chemical research over the past four decades. [1-3] For instance, due to the high electron affinity and superior to transport charge effectively, FDs can be used as effective acceptor compartments for organic photovoltaic (OPV) cells. Nowadays, OPVs have been concerned as a promising alternative technique for constructing inexpensive, clean and renewable energy sources due to their benefits such as low cost, decent mechanical performance and flexibility, and the opportunity of changing the chemical structure and producing effective devices in comparison with conventional inorganic semiconductor photovoltaic devices. The performance of OPVs is even more essential, as the production of inorganic photovoltaic cells is a source of extensive environmental pollution and energy consumption. Therefore, great research efforts aim at designing and synthesizing novel FDs as electron acceptors with better light-harvesting properties, higher electron mobility, and better miscibility with the polymer donor. However, the field of FDs properties still needs a lot of research, so that the usage of those species can be considered thoughtful and safe. In our approach, we attempt to extent this knowledge with the integrated use of computational chemistry methods and chemometric techniques.

The chemometric methodology to this matter based on the analysis of existing and computed data and the use of the analysis results for the systematization of knowledge or even for the prediction of physicochemical data of FDs for which experimentally determined values have been unavailable. In this contribution, we primarily focus on the relationship between the structural features and unique electronic properties of FDs. In particular, we have focused on four different physicochemical properties: the open-circuit voltage (V_{oc}) of solar cells comprising FDs, short-circuit current density (J_{SC}) of OPVs with FDs, solubility in common organic solvents (S) and the power conversion efficiency of the FDs' photovoltaic devices (PCE), and their relationship with the FDs' structure.

Performing chemometric analysis allow for determination a large amount of useful information and distinguish which aspect of the structure is responsible for the FD features or behavior of interest. Moreover, based on chemometric analysis assumption we can indicate the impact of FD structure modification on the power conversion efficiency of the photovoltaic devices. The capability of predefining FDs physicochemical properties can considerably reduce both costs and time of synthesizing new, safe and well perform the photovoltaic devices comprising C_{60} fullerene derivatives as acceptors of electrons. Finally, the knowledge that can be achieved as a result of theoretical estimation can considerably affect the process of designing new, safer OPVS, with properties more accurately corresponding to users requirements.

In this contribution, we develop a simple tool for the determination of FD features based on their molecular structures Information delivered by our tool can be further used in the considerations about particular FDs' application and safety.

Acknowledgment

This work was supported by the Polish National Science Centre (NCN) Grant No. NCN UMO-2012/07/D/NZ7/04342.

References

[1] C. Sikorska, "When a nanoparticle meets a superhalogen: a case study with C-60 fullerene," *Physical Chemistry Chemical Physics*, vol. 18, pp. 18739-18749, 2016.

[2] C. Sikorska, A. Gajewicz, P. Urbaszek, L. Lubinski, and T. Puzyn, "Efficient way of designing fullerene derivatives based on simplified DFT calculations and QSPR modeling," *Chemometrics and Intelligent Laboratory Systems*, vol. 152, pp. 125-133, 2016.

[3] C. Sikorska and T. Puzyn, "The performance of selected semi-empirical and DFT methods in studying C-60 fullerene derivatives," *Nanotechnology*, vol. 26, 2015.