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Towards designing polymers for photovoltaic applications: a DFT and experimental study of polyazomethines with various chemical structures

Jacek Wojtkiewicz[1*], Agnieszka Iwan[2*], Marek Pilch[1], Bartosz Boharewicz[2], Kamil Wójcik[2], Igor Tazbir[2], Maria Kaminska[1]

[1]*Faculty of Physics, University of Warsaw, ul. Pasteura 5, 02-093 Warsaw, Poland, [*]e-mail: wjacek@fuw.edu.pl*

[2]*Electrotechnical Institute, Division of Electrotechnology and Materials Science, M. Sklodowskiej-Curie 55/61 Street, 50-369 Wroclaw, Poland, [*]e-mail: a.iwan@iel.wroc.pl*

Abstract

Theoretical studies of polyazomethines (PAZs) with various chemical structures designated for photovoltaic applications are presented. PAZ energy levels and optical properties were calculated within density-functional theory (DFT and TDDFT) framework for 28 oligomers (monomer, dimer and trimer) of PAZs. The correlations between chemical structure of PAZ and location of its highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energy levels were examined. It turned out that the presence of triaminophenylene, dimethoxydiphenylene and fluorine group raises the orbital energies. As a consequence, it is a factor which improves the photovoltaic efficiency of solar cell built on the base of the corresponding PAZ and [6,6]-phenyl C_{61} butyric acid methyl ester (PCBM). On the contrary, quinone, 1,3,5-triazine and perfluorophenylene groups lower orbital energies and have negative influence on the photovoltaic efficiency. Moreover, calculations for methyl, ethyl and butyl analogs of P3HT as well as polythiophenes were performed and compared with the results obtained for PAZs. In addition experimental data are presented, which cover optical, electrochemical and electrical transport properties of the studied PAZs, allowing to determine HOMO and LUMO energies of the polymers and their conductivity. Finally, comparison between calculated and experimental results were made and discussed.