Ferroelectric Organic Layers on Graphene for Photovoltaics

Małgorzata Wawrzyniak-Adamczewska,[1] Paweł Masiak,[2]
Juan José Meléndez,[3] and Małgorzata Wierzbowska[4]

[1] *Faculty of Physics, Adam Mickiewicz University, Poznań, Poland*
[2] *Institut of Physics, Polish Academy of Sciences, Warszawa, Poland*
[3] *Department of Physics and Institute for Advanced Scientific Computing of Extremadura, University of Extremadura, Badajoz, Spain*
[4] *Institute of High Pressure Physics, Polish Academy of Sciences, Sokołowska 29/37, 01-142 Warsaw, Poland*

The electronic and optical properties of the aromatic molecules terminated with the dipole groups are studied within the DFT approach. The systems are simultaneously of donor and acceptor type. The path-separation for the electrons and holes is observed and the carrier mobilities are very high, as for the organic crystals. The band gap and the absorption spectrum can be tuned by changing a number of the aromatic rings. The physisorption process on the grephene causes the molecular distortions, and this leads to articulated change of the optical spectra.

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