The influence of salt on the polymeric semiconductor electronic structure in the active layer of polymeric light emitting electrochemical cells.

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Polymer light emitting electrochemical cells (PLECs) are organic electronic devices that are an alternative to the manufacture of organic light-emitting devices. However, until now some of the basic operational mechanisms involved in their operation of are not fully understood. Indeed it is well known that specific interactions involving the semiconducting polymer and ionic salts play an important role on the charge transport in the system. However details associated with this interaction are not understood yet. In this context, here we report a theoretical attempt to unravel some basic aspects on this subject. Structural and reactivity properties of the semiconducting polymer poly[(9,9-dioctylfluorenyl-2,7-diyl)-co-(1,4-vinylenebenzene)] and triflate lithium salt were evaluated via electronic structure calculations employing Parametric Method 6 (PM6) semi-empirical approach and Density Functional Theory (using B3LYP exchange-correlation functional and 6-31G basis set). Condensed-to-atoms Fukui indexes were evaluated by using Hirshfeld partition charge to identify preferred sites for polymer-salt interactions. The obtained results suggest that the presence of the ionic salt induces significant changes on electronic properties of the semiconducting polymer, which is dependent on the salt relative density and oxidation state, that facilitate the charge injection and transport in the devices. Acknowledgements: CNPq (Proc. 448310/2014-7), CNPq/PosMat/Unesp, Fapesp (2014/20410-1), Center for Scientific Computing (NCC/GridUNESP) of the São Paulo State University (UNESP).