Electropolymerization of 3 ',4 '-disubstituted 2,2 ':5 ',2 ''-terthiophene derivatives. A theoretical and photovoltaic characterization

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Abstract

In the present work a series of β-substituted thiophenes have been synthesized and their electrochemical behavior studied. The products obtained by electro-oxidation are highly dependent on the substituent, affording sometimes conducting polymers, insulating layers or soluble species. This behavior has been ascribed to specific electronic and/or steric factors. Theoretical calculations at the density functional theory level confirm the experimental findings and assess the use of reactivity descriptors for modeling complex chemical systems with specific polymerization patterns. In particular, the analysis of the polymerization sites of terthiophene derivatives using the dual descriptor for chemical reactivity and selectivity allows one to predict the specific sites able for reaction and explains correctly the observed polymerization pattern.