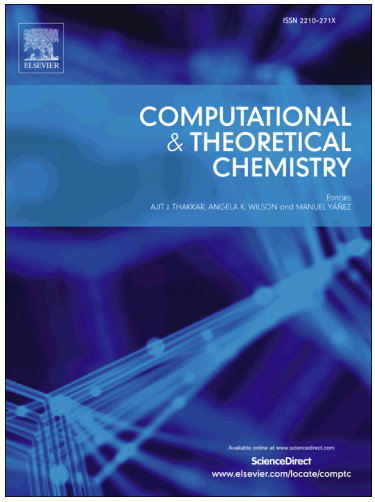

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Theoretical Studies on the Electronic Properties of Alkyl Chains

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ABSTRACT

The charge transfer of the alkyl chains was studied by density functional theory calculations at the B3LYP/6-311++G** level. Two different series of the saturated hydrocarbon chains, $C_nH_{2n+1}OH$ (n=10, 12, 14, 16, 18) and $C_{12}H_{25}X$ (X=–Cl, –OH, $–NH_2$) were considered for examining the effects of the chain length as well as the end group on the charge transfer properties of the alkyl chains. Computational results show that end group plays a key role on the electronic structures (HOMO-LUMO gap) of the saturated hydrocarbon chains, while the effect of the chain length on the conductive character of the alkyl chain is negligible. This is consistent with our previous experimental results. Further mechanism analysis of the charge transfer in saturated hydrocarbon chains indicates that HOMO-LUMO gap values depend strongly on the adiabatic ionization potentials (AIPs). Moreover, detailed spin density distribution analysis shows the radical cationic state is localized on the transport channel of the molecular orbital used for charge transfer.

Keywords: Saturated Hydrocarbon Chains: Charge Transfer: Adiabatic Ionization Potentials: Spin Density Isosurface: Density Functional Theory

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