

This thesis concerns with 4 basic aspects of the charge carrier transport: (1) depth of the potential well formed around the charge carrier when localized on a polymer chain; i.e. so called polaron binding energy. (2) Extent of the charge carrier delocalization over the polymer chain and influence of steric effects on this value. (3) Intrachain mobility of the charge carrier. (4) Effect of charge carrier transfer on the chain stability. Polysilanes, which are well known for their semi-conducting properties, were chosen as model material for investigation. Outlined properties were studied by means of quantum chemistry and molecular dynamics, which allowed us to investigate the process of the charge carrier transfer in great detail. Theoretical results were then compared to the experiments with very good agreement.