215. Title: Charge carrier mobility in poly[methyl(phenyl)silylene] studied by time-resolved terahertz spectroscopy and molecular modelling

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Abstract: Time-resolved terahertz spectroscopy and combination of quantum chemistry modeling and molecular dynamics simulations were used for the determination of charge carrier mobility in poly[methyl(phenyl)silylene]. Using time-resolved THz spectroscopy we established the on-chain charge carrier drift mobility in PMPSi as 0.02 cm(2) V (1) s (1). This value is low due to the formation of polarons: the hole is self-trapped in a potential formed by local chain distortion and the transient THz conductivity spectra show signatures of its oscillations within this potential well. This view is supported by the agreement between experimental and calculated values of the on-chain charge carrier mobility.