Summary in English

The aim of my doctoral dissertation was to investigate the influence of high pressure and temperature changes on the structure and photophysical properties of selected organic semiconductors, in order to deepen the understanding of the structure–property relationships in this group of compounds. The research was inspired by numerous literature reports on perovskite materials, which have shown that extreme conditions provide an effective tool for analyzing phase transition mechanisms and the relationship between structure and properties. However, in the case of organic semiconductors, this approach is still rarely applied, even though these materials play an increasingly important role in the development of modern photovoltaic and optoelectronic technologies.

The dissertation comprises a series of four articles presenting the results of studies on six selected organic semiconductors: the polymer PTB7 and small-molecule perylene diimide (PDI) derivatives with different substituents at the imide position. I correlated the structural analyses, conducted using X-ray diffraction, with UV-Vis-NIR and photoluminescence spectroscopy measurements, which enabled the identification and detailed characterization of several new polymorphs. The results revealed that variations in pressure or temperature induce significant changes in π–π stacking distances between aromatic cores, the conformation of the molecules, and their aggregation behavior. These structural modifications directly influence the band gap energy and the luminescent properties of the investigated materials.

In article **A1**, I presented the results of studies on PTCDI-Ph, a PDI derivative with phenyl substituents, for which I identified three polymorphs: one stable at ambient conditions, a high-temperature phase occurring above 493 K, and a high-pressure phase above 3 GPa. I observed reversible bathochromic shifts and changes in photoluminescence intensity that were dependent on pressure and temperature, indicating the potential of PTCDI-Ph as an active material in multimodal sensors. Article **A2** focuses on PDI-C_6, a derivative with N-substituted *n*-hexyl groups, for which I identified five polymorphs, including two high-pressure and two high-temperature phases. I demonstrated that pressure induces gradual conformational changes in the alkyl chains, while high temperature additionally causes rotations of the perylene cores. Article **A3** analyzes the PDI-C_n series (where n = 5–8) with alkyl substituents (C_nH_{2n+1}) of varying length. Using high-pressure single-crystal X-ray diffraction, I identified new phases and

correlated the obtained structural data with the observed shifts in the UV-Vis-NIR absorption and emission spectra. Article **A4** presents results on the polymer PTB7, with particular emphasis on the effects of high pressure and film preparation methods on its optical properties. I demonstrated that increasing pressure causes a bathochromic shift of the absorption edge and a narrowing of the band gap (E_g).

The conducted studies demonstrated that the use of extreme conditions provides an effective tool for modeling structural changes that directly influence fundamental properties of organic materials, such as band gap and luminescence. These results not only provide new insights into the behavior of organic semiconductors under high pressure and variable temperature but also highlight the possibility of tuning their optical properties through controlled structural modifications.