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The main goal of my dissertation was searching the molecular disorder for the selected model compounds in the solid-state. Nuclear Magnetic Resonance (NMR) spectroscopy and Density Functional Theory calculations (DFT) were used as the leading techniques. Employing these methods, I proved the power of the complementary approach in study of the condensed matter.

Six original papers collected as PhD thesis were published between 2012 and 2015. In these PhD projects I tested the available quantum chemical calculation methods on DFT level which today represent a standard procedures for liquid state NMR. As I revealed, data obtained employing this approach well, although not perfectly, correlate with experimental results for the solid state. Additionally, I applied the new method, GIPAW (*Gauge Including Projector Augmented Waves*) which recently is commonly used by NMR community, for theoretical calculations of condensed matter due to possibility to take into account periodicity of the crystal structure.

As experimental methods, I used NMR spectroscopy which is a powerful technique in structure determination of solid-state phases. Solid state NMR (SS NMR) is widely used in several scientific fields ranging from solid state physics to molecular biology. In my projects I employed different SS NMR techniques, *e.g.* slow rotation (1 – 2 kHz) of samples under magic angle (MAS), as well as the so-called Very-Fast MAS NMR technique which lets speed up the rotation up to 65 kHz.

On the course of my studies, I proved that differences between experimental (NMR) and theoretical results may be used as a valuable source of the information about the disorder on the molecular level. I showed that the chemical shift anisotropy parameter *span* is the most diagnostic tool, which may be used as the criteria for the analysis of the local molecular dynamics. I highlighted this observation in most of the papers which are included into this dissertation.

As models for investigations I chose two groups of objects. The first one are opioid peptides (ie. natural products) and the second are the synthetic polymers, polylactide (PLA) and polyhedral oligomeric silsesquioxanes (POSS). Focusing attention on these two completely different objects, with low molecular weight (peptides) and high molecular weight (polymers), I extended the GIPAW technique applicability showing that this method is working fine not only for small compounds but also for macromolecular systems (to the best

of my knowledge, I used here this technique for the first time for the fine refinement of the crystal structure of the synthetic polymer).

The challenging question, which I have tried to answer during my work, is related with verification of quality and real improvement of theoretical results comparing GIPAW methodology and the standard DFT approach. As I concluded, the difference between GIPAW and DFT calculations is significant. Employing the former method the assignment of ^{13}C, ^{15}N as well as ^{1}H signals is more reliable. Good correlation between the theoretical and experimental results for NMR and GIPAW methods opens the new strategy in structural studies, which today is known as NMR Crystallography. In my papers, I showed that it is possible the fine refinement of the crystal and molecular structure for compounds for which the X-Ray data deposited in the crystallographic bases are of poor quality. The most spectacular results I obtained for structures with R-factor over 10%. It is worth to note that in the Cambridge Crystallographic Data Center (CCDC), there are approximately 25 000 deposited structures which belong to this group. Four out of six papers included into this dissertation deal with this problem.

In my PhD thesis I paid attention to the specific problems which are within the scope of interest of scientists dealing with natural products as well as chemistry of material. Working with selected models, I provided important structural information about their structure and dynamics. Hopefully, this approach will be general. The new methodologies may be applied for searching of systems not included in this dissertation, structural problems connected with molecular disorder.