

**DEVELOPMENT AND VALIDATION OF NEW METHOD FOR FAST ESTIMATION
OF RELATIVE STABILITY FOR POLYMORPHIC SYSTEMS**

ZAKŁAD CHEMII FIZYCZNEJ, WYDZIAŁ CHEMICZNY, PW

Kierujący pracą: dr inż. **Krzysztof Durka**

Opiekun naukowy: dr **Anna Hoser**

Afiliacja opiekuna naukowego: Wydział Chemii Uniwersytetu Warszawskiego

The aim of the project is to establish a new method for combining theoretical calculations with experimental X-ray diffraction data in order to obtain relative stabilities for polymorphic systems. Polymorphism is the occurrence of a compound in several crystal forms which have different conformation of molecules or different packing of molecules in the crystal lattice. Polymorphism is a very important phenomenon because polymorphs of the same substance exhibit different physicochemical properties (melting point, solubility etc.) and different biological activity, which is important for the pharmaceutical industry. Around 30% of drugs exhibit more than one polymorphic form, and it is important to be sure before the drug is released to the market, that all polymorphic forms are known, characterized and the one which is active is a stable one. Relative stabilities at given temperatures can be established by theoretical calculations, however, such calculations are very time-consuming. Moreover, it is difficult to calculate accurate contributions from vibrational enthalpy and entropy to relative stability. Those thermodynamic properties can be estimated from single crystal X-ray diffraction data.

A new approach, being developed by us, shall allow estimation of the relative stability of polymorphs in wide temperature and pressure ranges on the basis of a combination of theoretical force fields and DFT calculations with the data from X-ray diffraction experiments.

Proposed thesis involves:

1. Crystallization of polymorphic systems, single crystal diffraction measurements
2. Theoretical computations (force fields, DFT)
3. Elaboration of a method for estimation of relative stability of studied polymorphic systems

Temat przeznaczony jest dla:	Proszę zaznaczyć właściwe pola wstawiając w sąsiedniej komórce znak „X”	
studentów kierunku*	Biotechnologia **	
	Technologia Chemiczna	X
studentów studiów*	I stopnia – praca inżynierska	X
	II stopnia – praca magisterska	
Wyrażam zgodę na zamieszczenie streszczenia pracy dyplomowej w wirtualnym dziekanacie***		TAK