

<b>Course title</b> Wykład monograficzny - Chemia kwantowa anionów molekularnych/Monographic lecture - Quantum chemistry of molecular anio		<b>ECTS code</b> 13.3.0432	
<b>Name of unit administrating study</b> Faculty of Chemistry			
<b>Studies</b>			
<b>Field of study</b>	<b>Type</b>	<b>Form</b>	
Chemistry	Master	Full-time studies	
<b>Teaching staff</b> Prof. dr hab. Piotr Skurski			
<b>Forms of classes, the realization and number of hours</b>		<b>ECTS credits</b>	
<b>A. Forms of classes, in accordance with the UG Rector's regulations</b> lecture		classes 30 h tutorial classes 10 h. student's own work 35 h TOTAL: 75 h - 3 ECTS	
<b>B. The realization of activities</b> In-class learning			
<b>Number of hours</b> Lectures, 30 h			
<b>The academic cycle</b> Second year, winter semester			
<b>Type of course</b> obligatory		<b>Language of instruction</b> Polish	
<b>Teaching methods</b> Lectures supported by multimedia presentations		<b>Form and method of assessment and basic criteria for evaluation or examination requirements</b>	
		<b>A. Final evaluation, in accordance with the UG study regulations</b> oral exam (conversation)	
		<b>B. Assessment methods</b>	
		<b>C. The basic criteria for evaluation or exam requirements</b>  Passing the final oral exam covering the issues presented during the lectures.	
<b>Required courses and introductory requirements</b>			
<b>A. Formal requirements</b> : quantum chemistry			
<b>B. Prerequisites</b>  basic knowledge concerning chemical structure of molecules and chemical bonds			
<b>Aims of education</b> acquainting students with the basic knowledge concerning molecular anions – their classification, properties, and applications			

### **Course contents**

Electronic structure of molecular anions, most fundamental properties of molecular anions, classification of anions based on the potential responsible for an excess electron binding, various types of molecular anions: valence-bound anions, multipole-bound anions, metastable anions, multiply charged anions, cluster anions, double-Rydberg anions, solvated electrons. Modern theoretical methods used for studying molecular anions, the most recent discoveries concerning the subject.

The course will provide the knowledge about molecular anions in general and various types of negatively charged systems in particular. In addition, the proper selection of theoretical methods appropriate for studying certain types of anions will be explained. The course will also cover the problem of electronic, kinetic and thermodynamic stability of anions.

### **Bibliography of literature**

#### **A. Literature required to pass the course**

##### A.1. Literature used during classes:

Theoretical Prospects of Negative Ions, ed. J. Kalcher, Research Signpost, Trivandrum, 2002, An Introduction to Theoretical Chemistry, Jack Simons, Cambridge University Press, 2003.

##### A.2. Literature for individual studies :

Theoretical Prospects of Negative Ions, ed. J. Kalcher, Research Signpost, Trivandrum, 2002, An Introduction to Theoretical Chemistry, Jack Simons, Cambridge University Press, 2003.

### **Knowledge**

the student defines the basic types of anions and explains their stability by characterizing the most important interactions responsible for an excess electron binding; the student is capable of describing the most important theoretical methods utilized for studying negatively charged systems.

### **Social competence**

After the course, the students are expected to understand the necessity of further learning, they are also taught to approach the problems and formulate their opinions with caution and criticism. In addition, the students are expected to remain open-minded for new ideas.