THEORY OF CHEMICAL REACTIVITY.

The aim of the course is to present simple theoretical methods for the interpretation of chemical reactivity. It will make it possible to understand and predict the possible outcome of a given chemical reaction. The approach will be essentially practical that will allow the students to apply by themselves the theoretical methods to actual reactivity problems.

The course will discuss the following topics:

1) Basic concepts of quantum theory.
2) Applications of quantum theory to chemistry. The Hamiltonian operator, the Schrödinger equation and its solution by variation and perturbation methods.
3) Atomic orbitals and hybridization.
4) The two-center problem and the localized and delocalized chemical bonds. Molecular orbitals and molecular structure.
5) The Hückel (HMO) method in variation and perturbation approaches.
6) The free electron (FEMO), non-bonding orbital (NBMO) and linear combination of molecular orbital (LCMO) methods.
7) Orbital interactions in molecules. The anomeric effect, non-classical ions and cis-trans isomerization.
8) Applications of HMO theory to molecular properties.
9) Various approaches to chemical reactivity: the initial state, the frontier (Fukui) orbital and localization methods. The reactivity indices and the transition state.
10) Perturbation theory of different classes of chemical reactions.
11) Symmetry controlled reactions.
12) Soft and hard acids and bases (SHAB).
13) Structure-reactivity relationships.
14) Potential energy surfaces (PES).

Termin	Dzień tygodnia	Godzina	Miejsce
10.03.2014	**Poniedziałek**	**9.15 – 12.00**	**Minicentrum Konferencyjne (Luwr)**
11.03.2014	**Wtorek**	**9.15 – 12.00**	**Minicentrum Konferencyjne (Luwr)**
12.03.2014	**Środa**	**9.15 – 12.00**	**Minicentrum Konferencyjne (Luwr)**
13.03.2014	**Czwartek**	**9.15 – 12.00**	**Minicentrum Konferencyjne (Luwr)**
14.03.2014	**Piątek**	**9.15 – 12.00**	**Minicentrum Konferencyjne (Luwr)**