Corsi di Dottorato in Scienze Chimiche
A. A. 2017-2018

(1) Prof. Assunta MARROCCHI: Rischio chimico.
Corso da tenersi durante il mese di Dicembre 2017.

Programma:
Introduzione. Pericolo chimico e rischio chimico; Il rischio chimico industriale; Il rischio chimico negli ambienti di ricerca. Principali riferimenti normativi. Definizione di sostanza e preparato; Definizione di agenti chimici pericolosi; Classi di pericolo; Pericolosità e concentrazione dei preparati; Sostanze incompatibili; Simboli ed identificazioni di pericolo. Il concetto di esposizione agli agenti chimici. Il valore limite di esposizione (TLV).
Regolamento GHS/CLP.
Etichettatura di sostanze e preparati; Schede di sicurezza; Criticità delle schede di sicurezza dei preparati; Esempi e discussione critica per l'interpretazione delle schede di sicurezza.
Vie di assorbimento di agenti chimici. Parametri che influiscono sull'assorbimento.
La valutazione del rischio chimico. Cenni sulla gestione dei rifiuti chimici. Misure di prevenzione e protezione.

2) Proff. Filippo De Angelis, Leonardo Belpassi, Paola Belanzoni:
Advanced electronic structure and dynamics methods for molecules and materials.
Corso da tenersi durante il mese di giugno 2018.

Program:
1) Electronic structure calculation methods: Hartree-Fock, post Hartree-Fock, DFT.
2) Relativistic effects in electronic structure: Dirac equation and spin-orbit coupling.
3) Time-dependent DFT. UV-vis spectra and nonlinear optical properties.
4) Calculations of molecular properties: IR, EPR, UV-vis spectra.
5) Relativistic effects: observations and applications to molecular and material properties (IR, UV-vis spectra).
6) Ab initio molecular dynamics methods. Car-Parrinello method. Applications (examples).
7) Applications to materials and processes for energy.

3) Prof. Piergiorgio Casavecchia:
Frontiers in Molecular Reaction Dynamics
Corso da tenersi durante il mese di giugno 2018.

Program:
The course will focus on recent advances in our understanding of the mechanism and dynamics of elementary (bimolecular) reactions, including photodissociation (unimolecular) reactions, as made possible by strong progress in experimental techniques (mainly based on molecular beams and laser methods). After a general introduction to the field of molecular reaction dynamics, the advances and new insights permitted by the new techniques, especially when complemented by synergistic theoretical calculations of the dynamics on the underlying ab initio, full-dimensional potential energy surfaces, will be discussed with focus on the following topics:
1) State-to-state dynamics of three-atom reactions including the effect of reagent vibrational excitation (tunneling and resonance mediated reactions);
2) State-resolved dynamics of four-atom reactions;

3) State-resolved dynamics of polyatomic reactions [CH_4(and isotopologues) + X (X=H, F, Cl, OH)], including the effect of selective vibrational excitation of the reagent: mode selective and bond specific chemistry;
4) Dynamics of polyatomic multichannel reactions (including intersystem crossing effects), of fundamental and practical relevance (from combustion to astrochemistry).

4) Prof. Alceo Macchioni: Structure and Reactivity of Organometallic Catalysts as Disclosed by Advanced NMR Techniques.
Corso da tenersi nel mese di giugno 2018.

Program:
The focus of the course is on the application of NMR techniques for disclosing the structure of organometallic catalysts in connection with their reactivity, with particular attention to intermolecular interactions. After having recalled some basic principles of 1D and 2D NMR spectroscopy and catalytic cycles, the following advanced topics are faced: 1) Interactions in the second coordination sphere of a transition metal complex; 2) NMR techniques for investigating the supramolecular structure (NOE and DOSY NMR spectroscopies); 3) Supramolecular structure/reactivity correlation for: a) catalysts for olefin polymerization, b) catalysts for CO/olefin copolymerization, c) catalysts for transfer hydrogenation, d) metal dendrimeric species.