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FACULTAD DE CIENCIAS EXACTAS Y NATURALES
U.B.A.

1.- DEPARTAMENTO: Física

2.- CARRERA de : a) Licenciatura en: ORIENTACION:
b) Doctorado y/o Post-Grado en: Doctorado
c) Profesorado en:
d) Cursos Técnicos en Meteorología:
e) Cursos de Idiomas:

3.- 1er. CUATRIMESTRE/2do. CUATRIMESTRE Año: 24-7-2006 AL 28-7-2006

4.- Nº DE CODIGO DE CARRERA: 02

5.- MATERIA: 8va. Escuela J.J. Giambiagi - A.

6.- PUNTAJE PROPUESTO: 1 (uno) punto

7.- PLAN DE ESTUDIOS: 1987

8.- CARACTER DE LA MATERIA: Optativa.

9.- DURACION: 24-7-06 al 28-7-06

10.- HORAS DE CLASES SEMANALES: hs

a) Teóricas:	hs.	d) Seminarios:	hs.
b) Problemas:	hs.	e) Teórico-problemas:	hs.
c) Laboratorio :	hs.	f) Teórico-prácticas:	hs.
		g) Totales horas:	hs.

11.- CARGA HORARIA TOTAL: 40 hs.

12.- ASIGNATURAS CORRELATIVAS:

13.- FORMA DE EVALUACION: Examen Final

14.- PROGRAMA ANALITICO: (se adjunta)

15.- BIBLIOGRAFIA:

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FIRMA DIRECTOR:

FIRMA PROFESOR:

ACLARACION FIRMA: Dra. María Cristina Caputo

Dra. SILVINA M. PONCE DAWSON
DIRECTORA
DEPARTAMENTO DE FISICA

Adrián E. Roitberg

Department of Chemistry, University of Florida, United States.

"Molecular Modeling of Biomolecules"

This course will introduce the simulation and computer modelling methods commonly used in biochemistry and biophysics, with a focus on physical models to understand the behaviour of biomolecules at a molecular level. Standard force fields will be presented, as well as the fundamentals of molecular dynamics and Monte Carlo simulations. Recent applications concerning dynamics of proteins, DNA, and lipids, calculation of protein folding processes, binding constants, protein-drug interactions, properties of ion channels as well as a number of recent literature topics will be presented.

Nicola Marzari

Massachusetts Institute of Technology, Department of Materials Science and Engineering-DMSE, MIT, Boston; United States.

"Computational Materials Science"

Computational Material Science is dedicated to the development and application of "computer experiments" to understand the microscopic behavior of materials. Most of the work relies on extensive electronic-structure simulations to determine ab initio (or from scratch) the properties of a given system from an accurate description of its interacting electrons and nuclei. The fundamental quantum-mechanical nature of this approach, for which Kohn and Pople were awarded the Nobel prize in 1998, allows for a wide range of applications and for a predictive power that can augment or complement experimental observations. Typical problems in materials science such as embrittlement of grain boundaries, binding of small molecules to nanotube sensors to interdisciplinary work in surface chemistry and catalysis (selective oxidation of methane, water ordering on metal electrodes) will be discussed.

Gustavo Scuseria

Robert A. Welch Professor Department Of Chemistry Rice University Houston, Texas, United States

" DFT: New Exchange and correlation functionals applications"

Subjects:

- New correlation and exchange functionals in Density Functional Theory; TPSS, and hybrids TPSSh and HSE
- Calculation of band gaps and crystalline structures employing HSE.
- Importance of electronic localization.
- Theory of Dirac-Kroll-Hess: Relativistic effects in solids and molecules. Application in bond energies
- DFT optical spectra employing DFT: comparison of theory and experiments. Applications in semiconducting single-walled carbon nanotubes - Examples in systems of useful for technological applications: C₂O₂, ZnO, MnO.

The Lectures

- **Molecular Modeling of Biomolecules,**

by Adrian E. Roitberg,
Quantum Theory Project and Department of Chemistry, University of Florida
<http://www.qtp.ufl.edu>

- **Computational Materials Science**

by Nicola Marzari,
Department of Materials Science and Engineering, Massachusetts Institut
Technology, Boston
<http://dmse.mit.edu>

- **DFT: New Exchange and correlation functionals applications**

by Gustavo E. Scuseria,
Rice University Houston, Texas
<http://python.rice.edu/~guscus>

- **Relativistic Quantum Chemistry**

by Lucas Visscher,
Section Theoretical Chemistry, Vrije Universiteit
<http://www.chem.vu.nl/~visscher>

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References:

- * Hybrid density functional theory and the insulating gap of UO_2 , K. N. Kudin, G. E. Scuseria, and R. L. Martin, *Phys. Rev. Lett.* 89, 266402-4 (2002).
- * Climbing the density-functional ladder: Nonempirical metageneralized gradient approximation designed for molecules and solids, J. Tao, J. P. Perdew, V. N. Staroverov, and G. E. Scuseria, *Phys. Rev. Lett.* 91, 146401 (2003).
- * Comparative assessment of a new meta-GGA density functional: Molecules and hydrogen-bonded complexes, V. N. Staroverov, G. E. Scuseria, J. Tao, and J. P. Perdew, *J. Chem. Phys.* 119, 12129-12136 (2003), erratum 121, 11507 (2004).
- * Tests of a ladder of density functionals for bulk solids and surfaces, V. N. Staroverov, G. E. Scuseria, J. Tao, and J. P. Perdew, *Phys. Rev. B* 69, 075102 (2004).
- * Relativistic all-electron self consistent hybrid density functional calculations including scalar and spin-orbit effects, J. E. Peralta and G. E. Scuseria, *J. Chem. Phys.* 120, 5875-5881 (2004).
- * Assessment and validation of a screened Coulomb hybrid density functional, J. Heyd and G. E. Scuseria, *J. Chem. Phys.* 120, 7274-7280 (2004).
- * Efficient hybrid density functional calculations in solids: Assessment of the Heyd-Scuseria-Ernzerhof screened Coulomb hybrid functional, J. Heyd and G. E. Scuseria, *J. Chem. Phys.* 121, 1187-1192 (2004).
- * Effect of the Perdew-Zunger self-interaction correction on the thermochemical performance of approximate density functionals, O. A. Vydrov and G. E. Scuseria, *J. Chem. Phys.* 121, 8187-8193 (2004).
- * Lattice defects and magnetic ordering in plutonium oxides: A hybrid density functional theory study of strongly correlated materials, I. D. Prodan, J. A. Sordo, K. N. Kudin, G. E. Scuseria, and R. L. Martin, *J. Chem. Phys.* 123, 014703 (2005).
- * Density functional theory study of optical transitions in semiconducting single-walled carbon nanotubes, V. Barone, J. E. Peralta, M. Wert, J. Heyd, and G. E. Scuseria, *Nano Lett.* 5, 1621-1624 (2005).
- * Optical transitions in metallic single-walled carbon nanotubes, V. Barone, J. E. Peralta, and G. E. Scuseria, *Nano Lett.* in press.
- * Energy bandgaps and lattice parameters evaluated with the HSE screened hybrid functional, J. Heyd, F. E. Peralta, G. E. Scuseria, and R. L. Martin, *J. Chem. Phys.* in press.

Luuk Visscher

Section Theoretical Chemistry, Vrije Iniversiteit, Amsterdam, Holanda.

"Relativistic quantum chemistry"

In accurate electronic structure calculations of heavy atom containing systems at the ab initio level relativistic effects must be explicitly taken into account. The importance of heavy atom containing systems in practical applications and experimental work has been growing in the last years. For these reasons in the last decade there has been great effort to develop theoretical tools for dealing with relativistic effects in a systematic way. The aim of this research is to allow chemical systems containing heavy element atoms to become accessible for computational studies, thus complementing experimental research. Two main lines can be recognized in this field. On one hand, the development of methods based on four-component spinors and the Dirac equation, within both mean-field and correlated methods. On the second hand, quasi-relativistic approaches based on two-component spinors based on approximations of the Dirac equation. Relativistic quantum chemical methods for the analysis of heavy atom containing systems will become standard techniques in the near future. For this reason this important subject is included among the lectures of this Giambiagi school

The Workshop

- * *Interacciones molécula-superficie: el óxido de magnesio como catalizador modelo*

by **Norberto Castellani**

Dpto. de Física, Universidad Nacional del Sur, Bahía Blanca, Argentina.
<http://www.uns.edu.ar>

En general son ms popularmente conocidas las propiedades catalíticas de sistemas metálicos. Sin embargo, los catalizadores no-metálicos como sulfuros y óxidos son ampliamente utilizados con fines prácticos. El óxido de magnesio ha recibido una especial atención porque poseyendo una estructura relativamente sencilla del tipo C1Na y no poniendo en juego electrones de valencia de la capa d, permite estudiar los sitios activos óxido-reductores que habitualmente presentan los otros óxidos más complejos. En este seminario se exponen los resultados teóricos que se han obtenido mediante métodos de orbital molecular o métodos de bandas deslocalizadas en una serie de trabajos dedicados tanto a la estructura superficial del MgO como a la adsorción y la reacción de moléculas sobre este óxido. Se ver cómo los diferentes métodos de la mecánica cuántica y los diferentes modelos propuestos (clusters, slabs) nos ayudan a comprender de una manera complementaria el comportamiento de su superficie.

- * *Hybrid QM/MM Method to study electronic properties and Tautomeric processes in solution.*

by **Kaline Coutinho**

Institute of Physics, Univ. São Paulo, CP 66318, 05315-970, São Paulo, SP, Brazil.
<http://fge.if.usp.br>

The study of solvent effects in molecular properties became one of the central topics in theoretical molecular physics. There is now a large variety of theoretical models to deal with the interaction between the solute and the solvent. These use either some continuum models, where the solvent molecules are represented by its dielectric constant, or a discrete model where explicit solvent molecules are used. In this latter, some computer simulation, Monte Carlo or Molecular Dynamics, is used to obtain the structure of the liquid at a certain temperature. We address the problem for studying the solvent effect on electronic properties of molecular systems and the tautomeric processes using a procedure based on the sequential use of Monte Carlo (MC) simulation and Quantum Mechanics (QM). This treats the solute, the solvent and its interactions by quantum mechanics. We first generate super-molecular structures of the solute surrounded by the explicit solvent molecules, performing MC simulations. Next these are used in subsequent QM calculations to obtain statistically converged average electronic properties. Binding energy, dipole moment, shift in the electronic spectrum and free energy differences are reported for some organic molecules in explicit water environment.

Supported by CNPq, CAPES and FAPESP

* *Challenges in Scientific Computing in the 21st Century: Cyber Infrastructure (CI) for Molecular Sciences.*

by **Julio Facelli**

Center for High Performance Computing, University of Utah, Salt Lake City Utah
84112, US.

<http://www.chpc.utah.edu>

This talk describes the activities under development in the area of cyber infrastructure (CI) or e-Science for molecular science applications. These activities include research in areas that have not been traditionally used in computational chemistry, such as integration of instruments, data bases and simulation methods. These emerging computational environments will greatly facilitate the use of CI not only by the experts, but also by scientists that traditionally have not used computational methods. Also the integration of methods appropriate to solve problems with different physical and temporal scales has the promise to greatly facilitate multiscale simulations. While the advances in computing will continue to produce evolutionary advances in computational chemistry, the new CI applications have the potential to radically change how molecular sciences are performed. Examples of our work in CSEO, MGAC-Grid, PriMe and Combustión-CGA will be used to demonstrate emerging CI applications.

* *Aromaticity in Atomic Clusters*

by **Patricio Fuentealba**

Facultad de Ciencias - Universidad de Chile, Chile.

<http://fisica.ciencias.uchile.cl/>

The concept of aromaticity has played a central role in the development of chemistry. However, as many other chemical concepts, it is empirical, and there is no just one definition of it. Hence, from a theoretical point of view it is difficult to define and many aromaticity scales have been proposed. On the other hand, the concept has been recently extended to non organic molecules, especially to atomic clusters. In this presentation a new aromaticity scale, based on the Electron Localization Function (ELF), will be presented and used to predict the aromaticity of some atomic clusters.

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- * *Size effects in the quantum interferences of the electronic states in metallic nanoparticles: Its manifestation in the Nuclear Magnetic Resonance spectrum.*

by **Horacio M. Pastawski** -

LaNAIS de RMS- FaMAF- Univ. Nac. de Córdoba, Argentina.
<http://www.lanais.famaf.unc.edu.ar/>

In absence of strong symmetries, a metallic nanoparticle can be considered a three dimensional chaotic stadium where the electrons moves ergodically forming random quantum interferences (scars structure) [1]. In consequence, each nucleus sees a different electronic environment. In an external magnetic field this manifests, through the Pauli susceptibility, in a distribution of effective fields sensed by the magnetic nuclei, i.e. a distribution of Knight shifts of the NMR frequencies [2]. This is observed as an inhomogeneously broadened line shape which is a fingerprint of the particle structure. In this tutorial lecture, we model the fluctuations in the local density of states for s electrons at the Fermi energy in a simple linear combination of atomic orbitals model. We will show how the LDOS is evaluated through to a matrix continued fractions calculation of the Green's functions. The simplest models, assume a chaotic nature [3] for electronics states and lead to universal scaling behavior with size and temperature, which describe reasonably the behavior of Cu and Pt [4]. However, the description of the smaller particles requires a further refinement [5, 6]: the consideration of shifts in the ionization energy of surface atoms with respect to bulk atoms. This leads to surface bands. Hence the projection of the electronic density of states on these sites presents two overlapping structures. One of them is characterized by the level spacing coming from bulk states and the other arises from the surface states. In very small particles, this effect contributes to an over-broadening of the NMR absorption spectra, determined by the Knight shift distribution of magnetic nuclei. We compare our calculated Knight shifts with experiments on aluminum nanoparticles, and show that the deviation of the scaling law as a function of temperature and particle size can be explained in terms of surface states [7].

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* *Modelado Molecular en Ciencias de Materiales y Sistemas Biológicos.*

by Reinaldo Pis Diez

CEQUINOR, Facultad de Ciencias Exactas, Universidad de la Plata, Argentina.

<http://www.quimica.unlp.edu.ar/cequinor/>

En el grupo de Química Teórica del CEQUINOR (UNLP) hemos estudiado una importante cantidad de sistemas que guardan relación con procesos de interés en Ciencia de Materiales y Ciencias de la Salud utilizando diversas herramientas que van desde simulaciones de dinámica molecular hasta cálculos de primeros principios basados en la teoría del funcional de la densidad.

En esta charla repasaremos brevemente dichos estudios que van desde propiedades estructurales y eléctricas de agregados de metales de transición y la interacción de zeolitas con pequeños hidrocarburos alifáticos, hasta la determinación de propiedades electrónicas en antiinflamatorios no esteroides y drogas de acción antitumoral.

* *Recent Developments in NMR and NQR Technology at Córdoba (Argentina)*

by Daniel Pusiol

SpinLock SRL, C. de Arenal 1020, Bo Rogelio Martínez, Córdoba, Argentina.

<http://www.spinlock.com.ar/bienvenido.htm>

Continuous Wave Magnetic Resonance (CWMR) has been used in the past as the principal procedure in NMR Spectroscopy. During the first years of the NMR, CW Spectrometers have been used, for instance, to select seeds of high oil content in a rapid and non-destructive way. After a long temporal passage through the Fourier Transformed Pulsed Spectrometers, a recent rediscovery of CW techniques has been produced. The new technology consists in applying successive short RF pulses to the sample so that the interference between the FID and the spin echo signals becomes constructive. After a short time interval needed to reach the stationary state imposed by the Continuous Wave Free Precession (CWFP) -or Steady State Free Precession SSFP- condition, many signals made up of FID and spin echo can be obtained. In this way rapid and accurate measurements can be reached. In this presentation we consider examples of applications Spin Echo, SSFP and CWFP procedures in Food and Petroleum Industries, as well as in Quadrupole Resonance based prohibited substances detectors.

Very fast (in the order of few seconds) measurements of the oil content in sunflower, where the calibration of the oil content vs. signal intensity depends on the oleic acid content, can be achieved by combining Spin-Echo and SSFP techniques. The multicomponent SSFP technique allows, in addition, a unique calibration curve for all cheeses produced in Argentina.

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For a number of reasons it is important to measure the oil production on line, at the well site. A number of devices are being used for this end. However, their reliability is poor, particularly regarding their precision and accuracy. The difficulties arise, essentially, from the fact that what comes out from the well is a variable and complex mixture of, mainly, oil, water and gas, and in different states of motion. CWFP Magnetic Resonance Technology seems to solve this problem in pipes with liquid production over hundred of cubic meters a day. We will shortly refer to an application of Relaxation Spectroscopy to determine the total and effective porosities in formation rock in our presentation.

Quadrupole Resonance is a bulk inspection technology for detecting crystalline explosive solids containing nitrogen-14 (^{14}N) nuclei such as RDX, TNT, and nitrates. NQR has been described as "an electromagnetic resonance screening technique" with the specificity of chemical spectroscopy. We will present our developments of Quadrupole Resonance Detectors applied to explosive detections in both luggage and the body.

* *Reaction Force. A Key Concept to Characterize Reaction Mechanisms*

by **Toro-Labbé**

Laboratorio de Química Teórica Computacional (QTC);
Facultad de Química, Pontificia Universidad Católica de Chile.
<http://www.puc.cl/quimica/>

The concept of the reaction force is presented and discussed in detail. For typical processes with energy barriers, it has a universal form which defines key points along an intrinsic reaction coordinate: the force minimum and maximum. The resulting regions along the reaction coordinate can be interpreted as involving preparation of reactants in the first, transition to products in the second, and relaxation in the third. This general picture is supported by the distinctive patterns of the variations in relevant global and local electronic properties such as chemical potential, hardness, charges and Fukui functions. Two important points that are brought out by the reaction force are (a) that the traditional activation energy is comprised of two separate contributions, and (b) that the transition state corresponds to a balance between the driving and retarding forces.

Toro-Labbé

- * *Computational chemistry in the study of pollutants produced in garbage incinerators, pulp mills and manufacturing industries: polychlorinated biphenyls, dibenzodioxins and dibenzofurans.*

by Oscar Ventura

Departamento de Experimentación y Teoría de la Estructura de la Materia y sus Aplicaciones.

Facultad de Química - Universidad de la República, Montevideo, Uruguay
<http://www.ccpq.fq.edu.uy>

Concern about the responsible use of the environment has been growing in the last two decades. Since Anastas and Warner book in 1998, green chemistry has been established as an emergent area of research, with clearly established goals and methods. Pollution prevention, main subject of the famous twelve principles of green chemistry, is today embodied in the recommendations of the US EPA and the European IPPC. Therefore, it is not surprising that it is being discussed also in our region. Very few has been done however on the systematic application of computational chemistry to aspects of pollution prevention and/or destruction, although papers do exist on areas closely related, like environmental or atmospheric chemistry. Since computational chemistry, especially in its quantum chemistry variety, may very well lead chemists to the use of atom economy (one of the core concepts in green chemistry) we think it is worthwhile to explore more full this interaction. We have thus started in our laboratory a program, which we call EcoCOP (Spanish acronym for Computational Studies on Persistent Organic Polluents), focused on the application of computational chemistry methods for the calculation of structural, thermochemical, kinetic, spectroscopic and reaction parameters of species involved in pollution processes. In this talk, I will describe some of the studies we have performed on chlorinated species involved in the production and bleaching of cellulose, presently a contentious issue in our region of the world, and some of the future work we are planning for the coming years.

