

J2IFAM 2012

IV Jornadas de Jóvenes Investigadores en Física Atómica y Molecular



February 1st – 3rd, 2012

Granada, Spain



UNIVERSIDAD DE GRANADA
FACULTAD DE CIENCIAS

Departamento de Física Atómica, Molecular y Nuclear



IV Jornadas de Jóvenes Investigadores en Física
Atómica y Molecular
(J2IFAM 2012)

Granada, February, 1st-3rd 2012

Sponsors and Supporters

We gratefully acknowledge the support of the following institutions:



Universidad de Granada



Grupo Especializado de
Física Atómica y Molecular



Facultad de Ciencias



Departamento de Física
Atómica, Molecular y Nuclear



Instituto Carlos I de Física
Teórica y Computacional

FisyMat

Programa Oficial de
Doctorado en Física y
Matemáticas

Programa Oficial de Doctorado en Física y Ciencias del Espacio

About J2IFAM

Introduction

Jornadas de Jóvenes Investigadores en Física Atómica y Molecular J2IFAM (Symposium of Young Researchers on Atomic and Molecular Physics) was created to allow graduate students and postdocs working in Spain to share their knowledge and discuss their recent research. The first edition took place in Madrid, in December 2008 and was organized by Departamento de Física Atómica, Molecular y de Agregados of Instituto de Física Fundamental (CSIC). The second edition of the meeting was held in January 2010 at Universitat de Barcelona. The third edition took place in February 2011 at Santiago de Compostela. The number of participants in the first edition was 18, it increased to 41 in the second edition and it was 31 in the third one. The current edition will take place at the Faculty of the Sciences of Granada and it is organized by the Department of Atomic, Molecular and Nuclear Physics of the University of Granada.

Conference Topics

- Physics of Aggregates
- Reaction Dynamics
- Quantum Chemistry
- Surface Physics
- Atomic and Molecular Collisions
- Ultracold Atoms and Molecules
- Nanomaterial Science
- Spectroscopy and Excited States
- Quantum Information
- Medical Physics
- Nuclear and Particle Physics

Organizers

The IV J2IFAM is organized by PhD Students and Post-docs at Departamento Física Atómica, Molecular y Nuclear from the Universidad de Granada

- Peter Alexander Bouvrie Morales
- Juan Manuel Cornejo García
- Ix-Berenice García Ferreira
- Wilfredo González Infantes
- Angel Guerrero Martínez
- Sheila López Rosa (currently at Universidad de Sevilla)
- Ana Majtey
- Rodrigo Navarro Pérez
- Juan José Omiste Romero
- Ignacio Luis Ruiz Simó

Scientific Program

Wednesday, February 1st

Hour	Speaker	Title
13:00 15:00	Registration	
15:00 15:25	Opening Session: GEFAM Vicepresident, Jesús Sánchez-Dehesa	
Sesion A. Chair: Ana Majtey		
15:30 15:55	Antonio Sánchez Coronilla	On the N-H hydrogen Bond
16:00 16:25	Juan José Omiste Romero	Theory of mixed-field orientation of linear molecules: Loss of adiabaticity
16:30 16:55	Elisa Isabel Martín Fernández	Cu(en) ₂ ²⁺ Molecular Dynamics: Classical vs. Ab Initio
17:00 17:30	Coffee Break	
Sesion B. Chair: Antonio Sánchez Coronilla		
17:30 17:55	Silvia Acosta Gutiérrez	Physical properties of small water clusters in low and moderate electric fields
18:00 18:25	Ana Majtey	The relationship between quantum entanglement and energy in two-electrons system
18:30 18:55	Peter Alexander Bouvrie Morales	The Generalized Quantum Similarity Index and the Geometric Rényi divergence: Applications to atomic densities
19:00 20:30	Posters session	

Thursday, February 2nd

Hour	Speaker	Title
Sesion C. Chair: Javier Rodríguez Díaz		
9:30 9:55	Garikoitz Balerdi Villanueva	Control of the CH ₃ I Predissociation at the Origin of the B Band
10:00 10:25	Marta González González	First observation of ground state I(² P _{3/2}) atoms from the CH ₃ I photodissociation in the B-band
10:30 10:55	María Eugenia Corrales Castellanos	Radical effects on the femtodynamics of several alkyl iodides
11:00 11:30	Coffee Break	
Sesion D. Chair: Juan José Nogueira Pérez		
11:35 11:55	Javier Rodríguez Díaz	The role of the $\pi\sigma^*$ excited states in the photodissociation in biological chromophores
12:00 12:25	Juan Manuel Cornejo García	Detección de Corrientes inducidas por núcleos exóticos almacenados en vacío a baja energía
12:30 12:55	Ignacio Luis Ruiz Simó	Strangeness production in neutrino reactions
13:00 14:00	Lunch	
14:30 18:00	Guided visit to the Alhambra	
21:00	Conference dinner	

Friday, February 3rd

Hour	Speaker	Title
Sesion E. Chair: Martin Heimsoth		
9:30 9:55	Sheila López Rosa	Relativistics effects via LMC and Fisher-Shannon complexity measures
10:00 10:25	Rodrigo Navarro Pérez	Relativistic quantum mechanics and hypercritical fields
10:30 10:55	Ángel Guerrero Martínez	Medidas de complejidad
11:00 11:30	Coffee Break	
Sesion F. Chair: María Eugenia Corrales Castellanos		
11:30 11:55	Juan José Nogueira Pérez	Classical trajectory simulations of gas-surface collisions
12:00 12:25	Alba Campo Cacharrón	Study of Cation... π Interactions Modulated by the Environment
12:30 12:55	Marcos Rellán	Metals interactions with corannulene
13:00 15:30	Lunch	
Sesion G. Chair: Juan José Omiste Romero		
15:30 15:55	Martin Heimsoth	Orbital Josephson Effect in driven Bose-Einstein Condensates
16:00 16:25	Ix-Berenice García Ferreira	Monte Carlo simulation of a medical linear accelerator: A comparative study of Geant3, PENELOPE and Geant4
16:30 16:55	Wilfredo González Infantes	Fluence and energy espectra for photon beams: A Monte Carlo study
17:00 17:25	Concluding remarks	

Poster Session

Wednesday, February 1st 19:00-20:30

Poster	Author	Title
P1	Peter Alexander Bouvrie and Ana Majtey	Quantum entanglement in exactly soluble atomic models: The Moshinsky models with three electrons, and with two electrons in a uniform magnetic field
P2	Antonio Sánchez Coronilla	AIM and ELF Analysis of azo-aromatic dimers
P3	Antonio Sánchez Coronilla	Solar Cell Dyes Topological Analysis
P4	Marcos Rellán Piñeiro	Cation binding in a curved surface
P5	María Jadraque	Charge-transfer processes in the assembly of neutral Si_nO_m silicon oxide clusters
P6	Elisa Isabel Martín	Theoretical Bjerrum length of PAH/PSS Polyelectrolyte Bilayers
P7	Juan Manuel Cornejo	Haces monoenergéticos de electrones para física fundamental y aplicaciones
P8	Jesús Sánchez Márquez	Pseudopotentials vs all electron, study applied to solar cells dyes calculations
P9	Adrián Ayala-Gómez	Study of the critical solutions of Dyson-Schwinger equations at infrared region
P10	Hubert Cybulski	Theoretical study of the pyridine-(helium) $_n$, $n = 1, 2$, van der Waals complexes

Abstracts

Oral Presentations

On the N-H hydrogen Bond

A. Sánchez-Coronilla

Departamento de Química Física. Facultad de Ciencias. Universidad de Cádiz

E-mail: antonio.coronilla@uca.es

The reactivity of the intra- and intermolecular hydrogen bonded systems has been attracting considerable attention in the last years due to its great interest in the photochemistry field. One of the most challenging problems in this field is the study of hydrogen bond interactions in molecules possessing both proton acceptor and donor centres.

The pyridine and pyrrole rings are the structural units of numerous naturally occurring alkaloids which possess a wide range of biological and pharmacological properties. In the present communication the perspective of comparative theoretical and experimental results on molecules with those chromophores is presented. Therefore, the spectral and photophysical analysis show the formation of intra- or intermolecular hydrogen bonds. These results have been used as a clue to theoretically scrutinize the geometries of these complexes. In order to get an improved knowledge of these hydrogen bonded complexes we have applied the Quantum Theory of Atoms in MoleculesTM, QTAIM [1], to localize bond critical points and to analyze the relationships between their locations and characteristics of the complexes also addressed through the Molecular Electrostatic Potential, MEP, mapping.

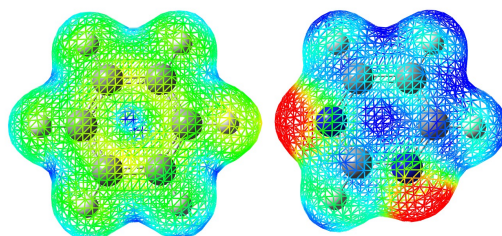


Figure 1: MEP mapping of Pyrimidine and benzene hydrogen bond interaction. Isovalue ($-1e^{-3}$ to 0.1)

[1] Bader, R. F. W., Atoms in Molecules. A Quantum Theory, Clarendon Press, Oxford (1994).

Theory of mixed-field orientation of linear molecules: Loss of adiabaticity

J. J. Omiste¹, R. González-Férez¹

¹*Física Teórica y Computacional, and Departamento de Física Atómica, Molecular y Nuclear,
Universidad de Granada, 18071 Granada, Spain
E-mail: omiste@ugr.es*

We present a theoretical study of mixed-field-orientation experiments of polar linear molecules. In these experiments, pendular states were created by means of linearly polarized strong laser pulses combined with tilted weak electric fields. Within the rigid rotor approximation, we assume that the dc field couples with the dipole moment and the ac field by means of the polarizability anisotropy, and solve the time-dependent Schrödinger equation taking into account the time profile of the alignment pulse. Our results show that the adiabaticity of the mixed-field orientation depends on the avoided crossings that the states suffer, as well as, on the formation on the quasidegenerate doublets that characterize the pendular regime. Hence, we probe that, in general, the weak dc field orientation is not adiabatic and that a time-dependent description of this process is mandatory. Specifically, we compare our numerical results with the measurements corresponding to the OCS molecule for different field configurations obtaining a good agreement [1]. This work complements our previous study for asymmetric top molecules exposed to tilted fields [2], where we have shown that an adiabatic description is not enough to explain the experimental results even for long laser pulses.

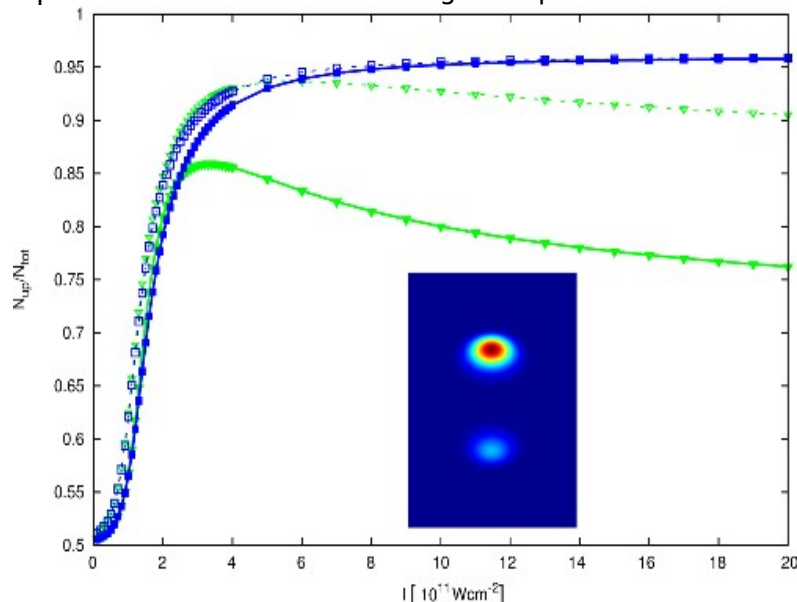


Figure 1: Orientation as a function of the intensity of the align laser.

[1] D. Dimitrovski, M. Abu-samha, L. Bojer Madsen, F. Filsinger, G. Meijer, J. Küpper, L. Holmegaard, L. Kalhøj, J. H. Nielsen, and H. Stapelfeldt. *Phys. Rev. A*, **83**:023405 (2011).

[2] J. J. Omiste, M. Gärttner, P. Schmelcher, R. González-Férez, L. Holmegaard, J. H. Nielsen, H. Stapelfeldt, and J. Küpper. *Phys. Chem. Chem. Phys.*, **13**:18815–18824 (2011)

Cu(en)_2^{2+} Molecular Dynamics: Classical vs. *Ab Initio*

E.I. Martín

Departamento de Química Física. Universidad de Sevilla

E-mail: elisamf@us.es

An *ab initio* interaction potential for the system $\text{Cu(en)}_2^{2+}\text{-H}_2\text{O}$ based in quantum-chemical calculations has been developed. Because of flexibility of Cu(en)_2^{2+} an intramolecular potential was fixed according to the main normal modes of optimized structure at MP2 level using MDF pseudopotential for Cu and AUG-cc-pVDZ basis set for N, C and H atoms (Fig. 1). After that a thorough exploration of the potential energy surface (PES) involving the complex and a water molecule was done. An analytical site-site like function is then used to describe the interaction between the two units.

In order to clarify the hydration structure obtained by classical Molecular Dynamics, an *ab initio* simulation of $\text{Cu(en)}_2 + 80 \text{ H}_2\text{O}$ was carried out with the CASTEP code using p.w/PBE-D [1].

The radial distribution functions corresponding to Cu-water oxygen pairs obtained on both methods shown a different behaviour for the hydration around Cu. It was possible to observe an asymmetrical axial hydration by *ab initio* simulation due to the loss of an axial water molecule.

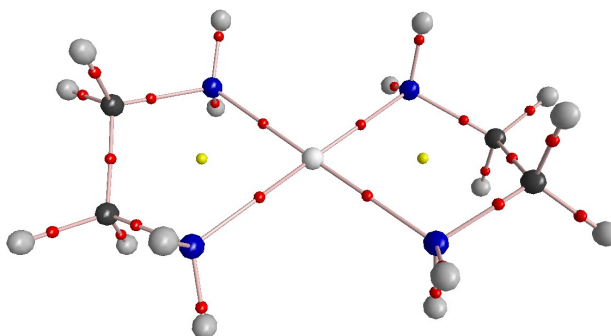


Figure 1: AIM analysis of the optimized structure at MP2 level for Cu(en)_2^{2+} .

[1] S. Grimme, J. Comp. Chem. 25, 1463 (2004).

Propiedades físicas de agregados de agua bajo la influencia de un campo eléctrico externo.

S. Acosta-Gutiérrez¹

¹ *Departamento de Física Fundamental II. Universidad de La Laguna. 38205 Tenerife.*

E-mail: silviaa.gutierrez@gmail.com

El conocimiento de la estructura geométrica y las energías de mínimo global para agregados de agua en diferentes entornos biológicos son importantes para la explicación y predicción de las observaciones experimentales. En particular los efectos de un campo eléctrico aplicado a un medio acuoso son relevantes no sólo en entornos biológicos sino también en otras aplicaciones científicas y tecnológicas.

En este trabajo se presentan las estructuras de mínimo global y el momento dipolar de agregados de agua $(\text{H}_2\text{O})_N$ ($2 \leq N \leq 20$), en presencia de un campo eléctrico externo. Analizaremos la importancia de los efectos de polarización en las estructuras de los agregados, comparando dos modelos de interacción semi-empíricos (TIP4P y Dang-Chang).

[1] S. Acosta-Gutiérrez, J. Hernández-Rojas, J. Bretón, J.M. Gómez Llorente and D.J. Wales, *J.Chem.Phys.* 135,124303 (2011).

The relationship between quantum entanglement and energy in two-electrons system

A.P. Majtey¹, A.R. Plastino^{1,2} and J.S. Dehesa¹

¹ *Instituto Carlos I de Física Teórica y Computacional y Departamento de Física Atómica, Molecular y Nuclear, Universidad de Granada, Granada 18071, Spain*

² *Universidad Nacional de La Plata, La Plata 1900, Argentina*

E-mail: anamajtey@ugr.es

The entanglement properties of two-electron atomic systems have been the subject of considerable research activity in recent years. These studies are still somewhat fragmentary, focusing on numerical computations on particular states of systems such as Helium, or on analytical studies of model-systems such as the Moshinsky atom. Some general trends are beginning to emerge from these studies: the amount of entanglement tends to increase with energy and, in the case of excited states, entanglement does not necessarily tend to zero in the limit of vanishing interaction between the two constituting particles [1,2]. A physical explanation of these properties, shared by the different two-electrons models investigated so far, is still lacking. It has recently been suggested that these features could be due to the particular entanglement measure employed [3].

As a first step towards an explanation, we consider here a perturbative approach to the analysis of entanglement in two-electrons models that sheds new light on the physical origin of the aforementioned features and on their universal character. In particular, this approach clarifies the fact that the second property mentioned above is independent of the entanglement measure used. In the case of the Moshinsky model, we also give an upper bound for the amount of entanglement in the limit of vanishing interaction in terms of the total energy of the system [4].

[1] R.J. Yañez, A.R. Plastino and J.S. Dehesa, Eur. Phys. J. D, **56**, 141 (2010).

[2] P.A. Bouvrie, A.P. Majtey, A.R. Plastino, P. Sánchez-Moreno, J.S. Dehesa, Eur. Phys. J. D in press (2011).

[3] M. Tichy, F. Mintert and A. Buchleitner, J. Phys. B, **44** 192001 (2011).

[4] A.P. Majtey, A.R. Plastino, J.S. Dehesa. Submitted 2011.

The Generalized Quantum Similarity Index and the Geometric Rényi divergence: Applications to atomic densities.

P.A. Bouvrie^{1,2}, J.C. Angulo^{1,2}, and J. Antolín^{2,3}

¹*Departamento de Física Atómica, Molecular y nuclear, Universidad e Granada, 18071-Granada*

²*Instituto Carlos I de Física teórica y Computacional, Universidad e Granada, 18071-Granada*

³*Departamento de Física Aplicada, EUITIZ, Universidad de Zaragoza, 50018-Zaragoza, Spain*

E-mail: bouvrie@ugr.es

A Generalized Quantum Similarity Index $QSI^{(q)}$ is defined [1], quantifying the similarity among density functions. The generalization includes, as new features (i) comparison among an arbitrary number of functions, (ii) its ability to modify the relative contribution of different regions within the domain, and (iii) the possibility of assigning different weights to each function according to its relevance on the comparative procedure.

The similarity among atomic one-particle densities in both conjugated spaces, and the neutral-ization similarity in ionization processes are analyzed. The results are interpreted attending to shell-filling patterns, and also in terms of experimentally accessible quantities of relevance in ionization processes, showing the versatility and universality of this divergence.

An alternative Rényi divergence $GRD^{(q)}$ derived from the previous measure, is proposed to quantifying the discrepancy among general probability densities [2].

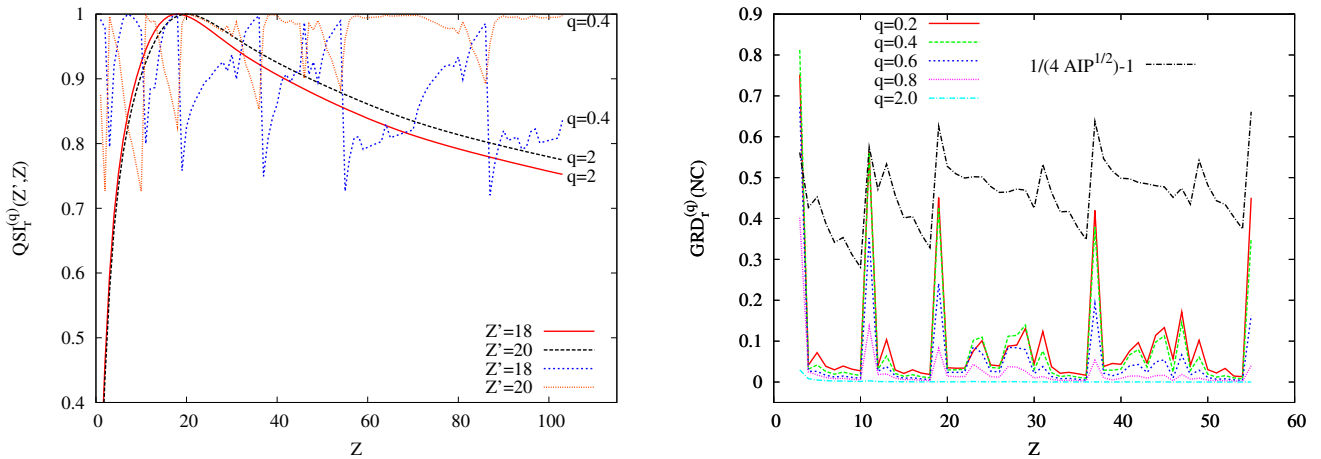


Figura 1: $QSI^{(q)}$ in position space among each of Argon $Z' = 18$ and Calcium $Z' = 20$ with respect to all neutral atoms, for $q = 0,4$ where we observe shellfilling patterns, and for $q = 2,0$ which is not observed (left). $GRD^{(q)}$ between a neutral atom (N) and its singly-charged cation (C) with $3 \leq Z \leq 55$ and the atomic ionization potential (AIP) of the neutral system. (Right).

[1] P.A. Bouvrie, J. Antolín, and J.C. Angulo, *Chem. Phys. Lett.* **506**, 326-331 (2011).

[2] J. Antolín, P. A. Bouvrie, and J. C. Angulo, *Phys. Rev. A* **84**, 032504 (2011).

Control of the CH₃I Predissociation at the Origin of the B Band

G. Balerdi¹, M. E. Corrales¹, G. Gitzinger^{1,2}, V. Loriot^{1,2}, R. de Nalda², and L. Bañares¹

¹*Departamento de Química Física I, Facultad de Ciencias Químicas, Universidad Complutense de Madrid, 28040 Madrid, Spain*

²*Instituto de Química Física Rocasolano, CSIC, C/Serrano 119, 28006 Madrid, Spain*
E-mail: garikoitz.bv@gmail.com

Predissociation of CH₃I after excitation at the origin of the B band (201.2 nm) occurs with a 1.5 ± 0.1 ps lifetime and almost only $I^*(^2P_{1/2})$ is generated [1]. However, when a control laser is temporally overlapped with the excitation pulse both quantum yield ($\Phi(I(^2P_{3/2})) = \frac{I(^2P_{3/2})}{I(^2P_{3/2}) + I^*(^2P_{1/2})}$) and predissociation lifetime can be modified.

Two different mechanisms change dissociation dynamics when a ~ 800 nm control laser is employed. Firstly, a new *pump-dump* channel is opened. Molecules are optically carried from the B band to a dissociative state that correlates with $I(^2P_{3/2})$ increasing its quantum yield. It also modifies the excited state lifetime by rapidly decreasing its population. In second place, as it has been proved [2], dynamic Stark effect can modify the dynamics of a chemical reaction. Specifically, in our molecule it shifts the B band energy potentially varying predissociation lifetime.

In this work, femtosecond laser pulses in combination with Velocity Map Imaging have been employed to measure this effects and a decrease in the B band lifetime to 0.8 ± 0.1 ps has been observed (Figure 1). The magnitude of the Stark shift was also measured for different control laser intensities.

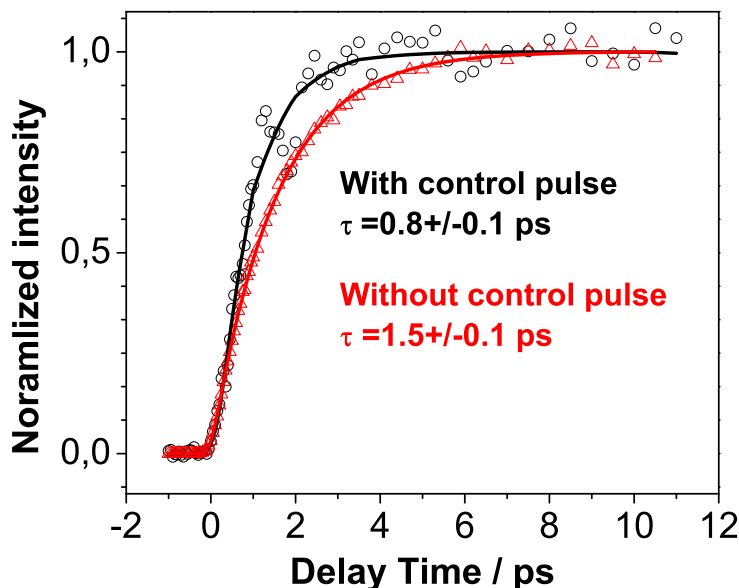


Figure 1: Integrated CH₃⁺ signal (from the CH₃I → CH₃($\nu=0$) + $I^*(^2P_{1/2})$ channel, after 2+1 REMPI ionization with a 333.45 nm probe laser) as a function of the pump-probe delay time with (black) and without (red) control pulse.

[1] G. Gitzinger, M.E. Corrales, V. Loriot, G.A. Amaral, R. de Nalda and L. Bañares, J. Chem. Phys. 132, 234313 (2010).

[2] B.J. Sussman, D. Townsend, M.Y. Ivanov and A. Stolow, Science 314, 278 (2006).

First observation of ground state $I(^2P_{3/2})$ atoms from the CH_3I photodissociation in the B -band

M. G. González¹, J. D. Rodríguez¹, L. Rubio-Lago¹, and L. Bañares¹

¹*Departamento de Química Física I, Facultad de Ciencias Químicas, Universidad Complutense de Madrid 28040 Madrid, Spain*

E-mail: marta.glezglez@hotmail.com

The photodissociation of CH_3I in the second absorption band (the B -band) has been studied at the wavelength 199.11 nm, coincident with the $3^1_0\ ^3R_1(E) \leftarrow X\ (^1A_1)$ CH_3I vibronic transition, using a combination of slice imaging and resonance enhanced multiphoton ionization detection of the CH_3 fragment. The kinetic energy and angular distributions of the recoiling CH_3 fragment confirm a major predissociation dynamics channel as a result of the interaction between the bound 3R_1 Rydberg state and the repulsive $^3A_1(E)$ state – ascribed to the A -band – yielding CH_3 fragments in correlation with spin-orbit excited $I^*(^2P_{1/2})$ atoms. In addition, first evidence of a non-negligible population of ground state $I(^2P_{3/2})$ atoms in the CH_3 fragment slice images, suggests a secondary predissociation mechanism via interaction between the 3R_1 Rydberg state and the repulsive A -band 1Q_1 state [1].

[1] M.G.González, J. D. Rodríguez, L. Rubio-Lago, and L. Bañares, The Journal of Chemical Physics, 135, (2011).

Radical effects on the femtodynamics of several alkyl iodides

M. E. Corrales^a, Gregory Gitzinger^{a,b}, Jesús González-Vázquez^{a,b},
Vincent Lorient^{a,b}, Rebeca de Nalda^b, Luis Bañares^{a*} and A. H. Zewail^c

^a *Departamento de Química Física I, Facultad de Ciencias Químicas,
Universidad Complutense de Madrid, 28040 Madrid, Spain*

^b *Instituto de Química Física Rosicolano, CSIC,
C/ Serrano 119, 28006 Madrid, Spain and*

^c *Physical Biology Center of Ultrafast Science and Technology,
Arthur Amos Noyes Laboratory of Chemical Physics,
California Institute of Technology, Pasadena, CA 91125, USA*

Abstract

The time-resolved photodissociation dynamics of several alkyl iodides (CH₃I, C₂H₅I, n-C₃H₇I, i-C₃H₇I and t-C₄H₉I) near the maximum of absorption of the A-band has been investigated employing the velocity map imaging (VMI) technique in combination with femtosecond pump-probe experiments. After one-photon excitation at 268 nm, a time-delayed probe pulse ionizes resonantly the iodine fragments in both the ground I(²P_{3/2}) and spin-orbit excited I*(²P_{1/2}) states via (2+1) REMPI at 304.5 nm. Three optically active excited states, the ³Q₁, ³Q₀ and ¹Q₁, compose the A-band in the alkyl iodides. The initial excitation leaves the parent molecule into the ³Q₀ state, which adiabatically correlates with I*(²P_{1/2}). It is well established that the I(²P_{3/2}) fragment observed in the experiments is the result of a non-adiabatic transition at the conical intersection between the ³Q₀ and ¹Q₁ states [1]. The influence of the alkyl group radical on the fragment recoil translational energy, the angular distributions and the clocking times of the different reactive channels is determined. The results are interpreted in terms of the dynamical dependence of the ¹Q₁ ← ³Q₀ non-adiabatic curve crossing on the size and structure of the alkyl radical.

* E-mail: banares@quim.ucm.es

The role of the $\pi\sigma^*$ excited states in the photodissociation in biological chromophores

Rodríguez J.D.¹, González M.G.¹ Rubio-Lago¹, L. and Bañares L.¹

¹*Departamento de Química Física I, Facultad de Ciencias Químicas, Universidad Complutense de Madrid, 28040 Madrid, Spain*

E-mail: javier.rodriguez.diaz@quim.ucm.es

DNA bases and aromatic amino acids show similar photodissociation schemes, which are mainly governed by transition from the ground state to two excited states, a bright bound state, $^1\pi\pi^*$, and a dark dissociative state $^1\pi\sigma^*$, and the interaction between them.

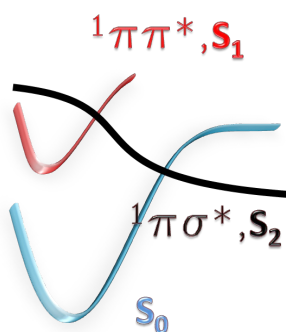
Different positions of the heteroatom in different aromatic rings change the energy of these states. The influence of the interaction between molecules can generate effects alike.

The effort carried out by different groups in the last few years to study a series of molecules with similar behavior but using different techniques has made it possible to reach a better understanding of the photodissociation of molecules that form living organisms.

A proper description of these processes may be the key to understand how life can be given under the extreme conditions of the universe and we might be able to discover the origin of some diseases.

In our laboratory we have determined that the role played by a dark state in the photodissociation changes noticeably with the molecular environment.

For this reason, we have designed a new type of experiment [1] in which we can control products and reagents to determine the solvent influence in the photodissociation of biomolecules, and thus to unravel how works the evasive $^1\pi\sigma^*$ state.



[1] L. Rubio-Lago, G. A. Amaral, A. N. Oldani, J. D. Rodríguez, M. G. González, G. A. Pino and L. Bañares, Phys. Chem. Chem. Phys., 13, 1082-1091, (2011).

Detección de Corrientes inducidas por núcleos exóticos almacenados en vacío a baja energía

J.M. Cornejo and D. Rodríguez

Departamento de Física Atómica Molecular y Nuclear, Universidad de Granada

E-mail: jmcg@ugr.es

Las trampas de iones magnéticas (trampas Penning) son actualmente los dispositivos que permiten medir las masas de iones atómicos con mayor precisión y exactitud. Un método de detección de iones utilizado en este tipo de trampas, es el conocido como Fourier-Transform Ion-Cyclotron-Resonance (FT-ICR) [1] que consiste en la determinación de la frecuencia de oscilación de un ion a partir de la corriente que éste induce de forma periódica en los electrodos de la trampa. En la Universidad de Granada se estudiará este sistema de detección, utilizando una trampa plana de dimensiones reducidas con un doble objetivo: 1) Su aplicación en la instalación SHIPTRAP sobre elementos superpesados [2] y cuyos resultados servirán para su implementación posterior en la futura instalación MATS (precise Measurements on very short-lived nuclei using an Advanced Trapping System) en FAIR [3], y 2) Calibración precisa del campo magnético producido por un dispositivo de creación de haces monoenergéticos de electrones a altas energías con aplicaciones al estudio de la función respuesta de detectores de radiación β u otros estudios en el campo de la física médica [4].

[1] M. Comisarow, J. Chem. Phys. 69, 4097 (1978)

[2] M. Block et al, Nature 463, 785-788 (2010)

[3] D. Rodríguez et al, Eur. Phys. J. ST 183, 1-123 (2010)

[4] J.M. Cornejo et al, este congreso

Strangeness production in neutrino reactions

M. Rafi Alam¹, I. Ruiz Simo^{2,3}, M. Sajjad Athar¹ and M.J. Vicente Vacas²

¹*Department of Physics, Aligarh Muslim University, Aligarh-202 002, India*

²*Departamento de Física Teórica and IFIC, Centro Mixto Universidad de Valencia-CSIC,
Institutos de Investigación de Paterna, E-46071 Valencia, Spain*

³*Departamento de Física Atómica, Molecular y Nuclear, Universidad de Granada, E-18071
Granada, Spain
E-mail: igruijsi@ific.uv.es*

We have studied charged current (CC) single kaon/antikaon production induced by either neutrinos or antineutrinos off free nucleons. Our model is based on the SU(3) chiral Lagrangians and resembles those used in pion production in the non-strange sector. Our cross sections results [1,2] could be of interest for the background estimation of various neutrino oscillation experiments like Mini-BooNE and SuperK. They can also be helpful for other planned neutrino experiments (MINER ν A, T2K phase II...) which are expected to study several strange particle production reactions with both neutrino and antineutrino beams with high statistics.

[1] M. Rafi Alam, I. Ruiz Simo, M. Sajjad Athar and M.J. Vicente Vacas, Physical Review D, Vol (82), 033001 (2010).

[2] M. Rafi Alam, I. Ruiz Simo, M. Sajjad Athar and M.J. Vicente Vacas, Physical Review D, Vol (85), 013014 (2012).

Relativistic effects via LMC and Fisher-Shannon complexity measures.

S. López-Rosa^{1,3}, P.A. Bouvrie^{2,3}, and J.S. Dehesa^{2,3}

¹*Departamento de Física Aplicada II, Universidad de Sevilla*

²*Departamento de Física Atómica, Molecular y Nuclear, Universidad de Granada*

³*Instituto Carlos I de Física Teórica y Computacional, Universidad de Granada*

E-mail: slopezrosa@us.es

We quantify relativistic effects of two different one-particle Coulomb systems (i.e. the pionic atom and hydrogenic systems) by means of single (Fisher information) and composite (Fisher-Shannon and LMC complexities) information-theoretic measures. While the Fisher information measures the gradient content of the density, the dimensionless composite information-theoretic quantities grasp two-fold facets of the electronic distribution: The Fisher-Shannon complexity measures the combined balance of the gradient content and the total extent of the electronic charge, and the LMC complexity quantifies the disequilibrium jointly with the spreading of the density in the configuration space. Opposite to other complexity notions (e.g., computational and algorithmic complexities) these two quantities describe intrinsic properties of the system because they do not depend on the context but they are functionals of the electron density. Moreover, they are closer to the intuitive notion of complexity, because they are minimum for the two extreme (or least complex) distributions of perfect order and maximum disorder.

It is observed that, contrary to the non-relativistic case, the complexity measures of these systems does depend on the potential strength (nuclear charge). In the case of the first system under consideration, i.e. the pionic atom described by the Klein-Gordon equations, its variation with the quantum numbers (n, l, m) is analysed in various ground and excited states; it is found that the relativistic effects enhance when n and/or l are decreasing [1]. For the Dirac hydrogenic systems, we can observe that the relativistic effects produce not only the well known compression-towards-the-origin of the electronic charge (also detected by the complexity measures in the pionic atom), but also a raising of all the non-relativistic minima of the electron density of the excited states of these systems which had not been realized up until now [2].

[1] D. Manzano, S. López-Rosa and J.S. Dehesa, EPL 90 (2010).

[2] P.A. Bouvrie, S. López-Rosa and J.S. Dehesa, preprint 2012

Relativistic quantum mechanics and hypercritical fields

R. Navarro Pérez¹, and E. Ruiz Arriola¹

¹*Departamento de Física Atómica, Molecular y Nuclear, Universidad de Granada, E-18071 Granada, Spain.*

E-mail: rnavarrop@ugr.es

We study the applicability of current conservation to relativistic quantum mechanical systems. This allows to set boundary conditions to the wavefunctions and resolve the singularity of imaginary energy that emerges from the Sommerfeld approximation for a strong Coulomb field. We focus on spin 0, 1/2 and 1 particles through Klein-Gordon, Dirac and Proca equations respectively. In the case of Dirac spinors current conservation is equivalent to hermicity of the Hamiltonian operator. Real valued energy spectra are obtained for the ground state and first excited states of Hydrogen like atoms as a function of the nucleus charge Z .

Medidas de Complejidad

A. Guerrero¹, P. Sánchez-Moreno² and J. S. Dehesa¹

¹ *Departamento de Física Atómica, Molecular y Nuclear, Universidad de Granada, España*

² *Departamento de Matemática Aplicada, Universidad de Granada, España*

E-mail: agmartinez@ugr.es

Las medidas de complejidad de Crámer-Rao, Fisher-Shannon y LMC (López-Ruíz, Mancini y Calvet) son calculadas en una dimensión utilizando el concepto de densidad de Rakhmanov de los polinomios ortogonales clásicos (Hermite, Laguerre y Jacobi) con respecto a la función peso correspondiente. Estas medidas dan una idea de cómo de compleja es la función en estudio (en el sentido intuitivo de la palabra complejidad) en el intervalo de ortogonalidad correspondiente. Posteriormente se generaliza el concepto de complejidad a dimensión 3, caso en el que se puede estudiar la complejidad de diversos sistemas atómicos ó sistemas cuánticos.

Classical trajectory simulations of gas/surface collisions

Juan José Nogueira¹, Emilio Martínez-Núñez¹ and Saulo A. Vázquez¹

¹ Departamento de Química Física and Centro Singular de Investigación en Química Biológica y Materiales Moleculares, Campus Vida, Universidad de Santiago de Compostela, 15782 Santiago de Compostela, Spain

E-mail: juanjose.perez1@rai.usc.es

Self-assembled monolayers (SAMs) have been widely investigated in the last years because of their attractive properties from a theoretical and experimental standpoint. Collisions of gases with SAMs permit to study a great variety of interesting processes [1-3]. Many microscopic characteristics of these gas/surface collisions cannot be observed and analyzed experimentally. The classical trajectory approach is a very useful theoretical technique because it yields an easy picture of the dynamics. In this work we provide a general analysis of CO₂/SAM and NO/SAM collision mechanisms.

[1] Cooks, R. G.; Ast, T.; Pradeep, T.; Wysocki, V. *Acc. Chem. Res.* 27, 316-23 (1994).

[2] Cooks, R. G.; Jo, S.-C.; Green, J. *Appl. Surf. Sci.* 231-232, 13-21 (2004).

[3] Gologan, B.; Green, J. R.; Alvarez, J.; Laskin, J.; Graham, C. R. *Phys. Chem. Chem. Phys.* 7, 1490-1500 (2005).

Study of Cation $\cdots\pi$ Interactions Modulated by the Environment

A. Campo-Cacharrón¹, A. A. Rodríguez-Sanz¹, E. M. Cabaleiro-Lago¹, J. Rodríguez-Otero²

¹*Departamento de Química-Física, Facultade de Ciencias, Universidade de Santiago de Compostela, Av. Alfonso X O Sabio s/n 27002, Lugo, SPAIN*

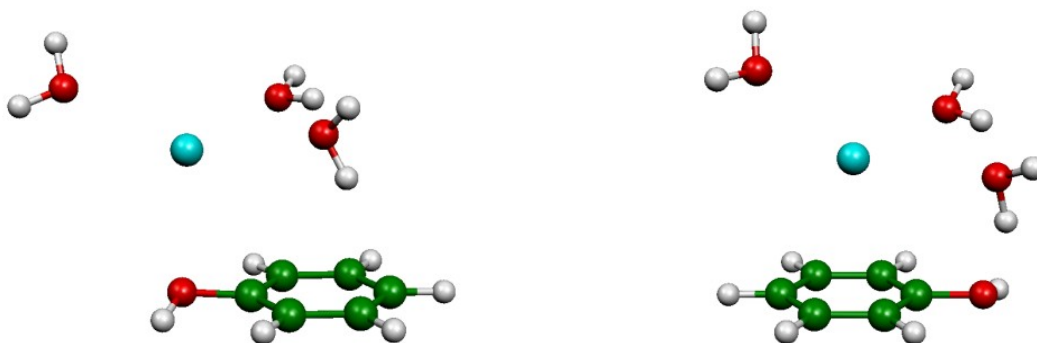
²*Departamento de Química-Física, Facultade de Química, Universidade de Santiago de Compostela, Av. das ciencias s/n 17582, Santiago de Compostela, SPAIN*

E-mail: alba.campo@usc.es

The cation $\cdots\pi$ interaction is a strong, general non-covalent binding force that is observed in a range of biological contexts like molecular recognition in biological receptors, enzymatic processes, etc. This kind of interactions has been mainly studied in gas phase where its behavior is clearly established, though in biological systems the aqueous environment is of the greatest importance. In fact, the presence of water molecules modulates the strength of the interaction between metal ions and aromatic species.

In the present work, a study of the interaction between simple cations and phenol has been carried out to shed light on the effect of successive hydration on the interaction. Phenol presents two coordination sites for cations: the aromatic ring and the hydroxyl oxygen, thus allowing a greater variety of structures to be formed than in benzene. Also, the hydroxyl group can be hydrated and participate in the formation of the hydrogen bond network.

So, ab initio and DFT methods were employed for studying the stepwise microhydration of phenol \cdots cation complexes, locating the most stable structures and obtaining the corresponding complexation energies. The results suggest that the participation of the hydroxyl group is already relevant in clusters containing a small number of water molecules.



Metals interactions with corannulene

Rellán Piñeiro¹, D. Josa¹, J. Rodríguez Otero¹, E. M. Cabaleiro Lago²

¹Centro de Investigación en Química Biolóxica e Materiais Moleculares (CIQUS), Universidade de Santiago de Compostela, Rúa Jenaro de la Fuente, s/n, Santiago de Compostela, 15782, SPAIN

²Departamento de Química Física, Universidade de Santiago de Compostela, Facultad de Ciencias, Avda. de Alfonso X o Sabio s/n, Lugo, 27002, SPAIN

E-mail: marcos.rellan@usc.es

In biological and molecular chemistry non-covalent interactions (hydrogen bonding, hydrophobic interactions, van der Waals interactions,..) are very important. They give structure and function of biological macromolecules. One of these non-covalent interactions is cation- π interaction, with a great importance in biological processes. The study of interactions with flat surfaces from benzene to graphite is a topic that has been very studied. In last years curved π surfaces, as fullerenes, have gained interest, and several studies on compounds with curved surfaces have been performed. The smallest example of curved π surface is corannulene, $C_{20}H_{10}$, which is the simplest buckyball. It is the smallest fragment of buckminsterfullerene, C_{60} .

To date, we have performed a work about the interaction of corannulene with alkali cations (Li^+ , Na^+ , K^+). The study was completed with DFT and MP2 methods, which gave some different results. Currently, we are carrying out a study with a ruthenium complex, being its interaction with corannulene different from that with fullerene. Other work that we are performing is the interaction of Fe^{2+} cation with two corannulenes, what can be seen as a structure derived from ferrocene.

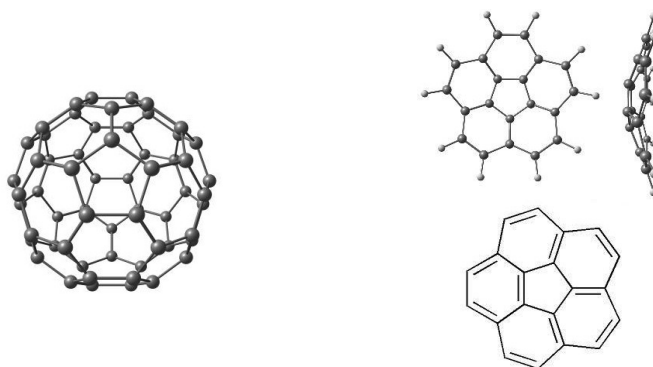


Figure 1.- Structure of fullerene and corannulene.

Orbital Josephson Effect in driven Bose-Einstein Condensates

M. Heimsoth^{1,2}, C. E. Creffield¹, L. D. Carr^{2,3}, and F. Sols¹

¹*Departamento de Física de Materiales, Universidad Complutense de Madrid, 28040 Madrid, Spain*

²*Department of Physics, Colorado School of Mines, Golden, Colorado 80401, USA*

³*Physikalisches Institut, Universität Heidelberg, Philosophenweg 12, 69120 Heidelberg, Germany*
E-mail: heimsoth@fis.ucm.es

We analyse the dynamics of Bose-Einstein Condensates (BECs) perturbed by a weak periodic driving field. Our main result is that (under certain conditions) the dynamic of such systems can effectively be described by a time independent few-mode Hamiltonian. This Hamiltonian reveals an analogy of these systems to those which feature the Josephson Effect (JE) in BECs. Hence, we regard this as a new manifestation of the JE in BECs, and term it the Orbital Josephson Effect [1]. We use our findings to study the rich dynamical behaviour of a hamiltonian quantum ratchet.

[1] M. Heimsoth, C. E. Creffield, L. D. Carr, F. Sols, arXiv:1112.5046.

Monte Carlo simulation of a medical linear accelerator: A comparative study of Geant3, PENELOPE and Geant4

Ix-B. García-Ferreira¹, R. Barrios¹, M. Vilches², A. M. Lallena¹, W. González¹ and M. Anguiano¹

¹ *Departamento de Física Atómica, Molecular y Nuclear, Universidad de Granada, E-18071 Granada, Spain*

² *Servicio de Radiofísica Hospital Universitario "San Cecilio", Avda. Dr. Olóriz 16, E-18012 Granada, Spain*

E-mail: ixbgf@ugr.es

The characterization of the dose distribution in water of an electron beam from a Siemens Mevatron KDS clinical linear accelerator (linac) was investigated by Monte Carlo (MC) simulation using the MC codes Geant3 [1], PENELOPE [2] and Geant4 [3] through GAMOS [4] framework. The entire geometry including the accelerator head and the water phantom was simulated to calculate the relative depth-dose distribution. Also the output factors were calculated by the three codes. In this work we present preliminary results of the simulations obtained with the three MC codes.

[1] GEANT, CERN Program Library Long Write-up, W5013 (1993).

[2] Salvat, F., et. al., NEA (2006).

[3] Agostinelli S., et. al., Nucl. Instrum. Methods Phys. Res. A, 506, 250- 303 (2003).

[4] Arce P., et al., IEEE Nucl. Sci. Conf. R., 3162-3168 (2008).

Fluence and energy spectra for photon beams: A Monte Carlo study

W. González, I.-B. García-Ferreira, M. Anguiano and A. M. Lallena

Departamento de Física Atómica, Molecular y Nuclear.

Universidad de Granada

E-mail: wgonzalez@ugr.es

Much of the algorithms used to calculate dose distributions for photon beams generated by clinical electron linacs consider three particle sources: a photon source corresponding to Bremsstrahlung in the target (primary source), a second photon source that takes into account those photons produced by scattering into the primary collimator, the flattening filter and the secondary collimation system (scattering source) and an contamination electron source that considers those electrons produced in the various components of the linac head and the air space between it and the patient (contamination electron source). In this work we aim at describing the source characteristics at the particular positions where particles originate. Source characteristics were studied within Monte Carlo simulation. To describe the photon fluence of the primary source, a phase space file was determined just below the target. The corresponding distribution was fitted by means of a Gaussian distribution or a Pearson distribution of order VII. The contribution of the scattering source was analyzed obtaining a phase space file just below the flattening filter. The corresponding fluence distribution can be fitted by means of a Gaussian specific for each linac head. The contamination electron source was analyzed by constructing a phase space file at the entrance of the secondary collimators. Using the particle directions at this position, the electron distribution is characterized below the flattening filter. An energy dependent Gaussian behavior was found for this third source. The energy spectrum of the primary source was analyzed with the phase space file determined below the flattening filter. In the beam axis, it was found that this energy spectrum can be fitted with a lognormal function. The photon energy for the scattering source can be obtained from that of the primary source assuming that scattered photons are generated by Compton interactions of the photons of the primary source with the head elements. This was verified using a phase space file, just below the flattening filter, in which the particle direction with respect to that of the particle that produced it is also scored.

Posters

Quantum entanglement in exactly soluble atomic models: The Moshinsky models with three electrons, and with two electrons in a uniform magnetic field

P.A. Bouvrie¹, A.P. Majtey¹, A.R. Plastino^{1,2}, P. Sánchez-Moreno³, and J.S. Dehesa¹

¹ *Instituto Carlos I de Física Teórica y Computacional y Departamento de Física Atómica, Molecular y Nuclear, Universidad de Granada, Granada 18071, Spain*

² *Universidad Nacional de La Plata, La Plata 1900, Argentina*

³ *Departamento de Matemática Aplicada, Universidad de Granada, Granada 18071, Spain*

E-mail: bouvrie@ugr.es

We investigate the entanglement properties of the eigenstates of a three-electron Moshinsky model. We analytically compute the amount of entanglement exhibited by the wavefunctions corresponding to the ground, first and second excited states of the system. We found that the amount of entanglement of the system tends to increase with energy, and in the case of excited states we found non vanishing entanglement in the limit of vanishing interaction. We also analyze the entanglement properties of the ground and some excited states of the two-electrons Moshinsky model in the presence of a magnetic field. We observe two main tendencies. On the one hand the amount of entanglement of the excited states does not vanish for weak interaction and on the other hand we show that for strong magnetic fields the entanglement reaches a finite value dependent on the interaction strength. For both, two and three electrons cases, we consider a perturbative approach in order to clarify the non vanishing entanglement of excited states in the limit of vanishing interaction. As far as we know this is the first work that provides analytical and exact results for the entanglement of the ground and the first few excited states in a three-electron model [1].

[1] P.A. Bouvrie, A.P. Majtey, A.R. Plastino, P. Sánchez-Moreno, J.S. Dehesa, Eur. Phys. J. D in press (2011).

AIM and ELF Analysis of azo-aromatic dimers

A. Sánchez-Coronilla¹, E.I. Martín²

¹ *Departamento de Química Física. Facultad de Ciencias. Universidad de Cádiz*

² *Departamento de Química Física. Universidad de Sevilla*

E-mail: antonio.coronilla@uca.es

In this communication we present theoretical results on hydrogen bond dimers of pyrrole and pyridine derivatives.

Changing the interacting molecules we have modulated the donor and acceptor capabilities in the dimers. The characteristic of the hydrogen bonds have been analysed by employing the Topological analysis of Quantum Theory of Atom in Molecules, QTAIM [1] and Electron Localization Function, ELF [2]. The results clearly show three different hydrogen bond interactions involving the nitrogen atoms in those molecules. Therefore, we found: a) two H-bond interactions of different strength along the Npyrrole-H-Npyridine bond path; b) a weak H-bond corresponding to the C-H-Npyridine bond path.

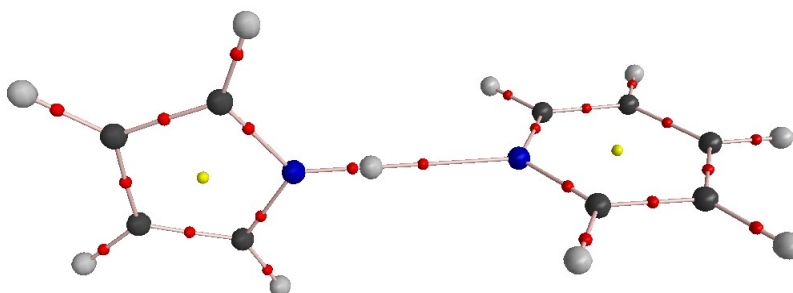


Figure 1: AIM analysis of pyrrole and pyridine hydrogen bond interaction

[1] Bader, R. F. W., *Atoms in Molecules. A Quantum Theory*, Clarendon Press, Oxford (1994).

[2] Becke, A.D.; Edgecombe, K.E., *J. Chem. Phys.*, 92, 5397-5403 (1990).

Solar Cell Dyes Topological Analysis

**A. Sánchez-Coronilla, J. Sánchez Márquez, D. Zorrilla, J. Navas, R. Alcántara,
C. Fernández-Lorenzo and J. Martín-Calleja**

Departamento de Química Física. Facultad de Ciencias. Universidad de Cádiz

E-mail: antonio.coronilla@uca.es

Experimental works on dyes solar cells, DSCs, show the effectiveness of Ruthenium-dyes as compared to other Metal-dyes [1]. On the basis of these experimental remarks, we present a theoretical study based on Ru-dyes of interest in solar cells.

Our principal interest is focussed to scrutinize the Ru role in the dyes. With this purpose in mind, the stability of the systems of increasing size has been studied. We have selected the complex of Ru with 6 pyridine molecules as a model to simulate the *cis*-Bis(isothiocyanato) bis(2,2'-bipyridyl-4,4'-dicarboxylato ruthenium (II) dye, **N3**. Topological analysis of Quantum Theory of Atom in Molecules, QTAIM [2], Electron Localization Function, ELF [3], and HOMO-LUMO analysis have been applied to test the stability of Ru-based complexes upon increasing the number of pyridine molecules (up to 6).

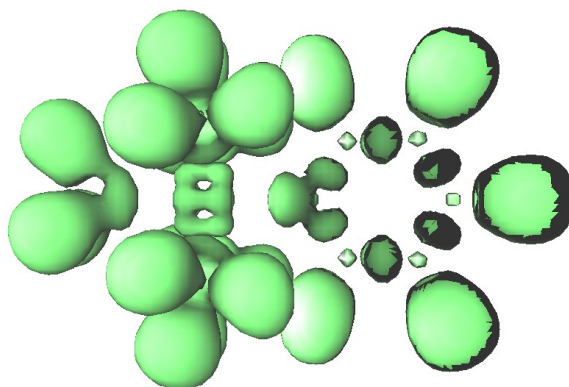


Figure 1: ELF of Ru-5NH₃-1Pyridine complex

[1] O'Reagan, B.; Grätzel, M., *Nature*, 353, 737-740 (1991).

[2] Bader, R. F. W., *Atoms in Molecules. A Quantum Theory*, Clarendon Press, Oxford (1994).

[3] Becke, A.D.; Edgecombe, K.E., *J. Chem. Phys.*, 92, 5397-5403 (1990).

Cation binding in a curved surface

M. Rellán Piñeiro¹, D. Josa¹, J. Rodríguez Otero¹, E. M. Cabaleiro Lago²

¹Centro de Investigación en Química Biolóxica e Materiais Moleculares (CIQUS), Universidade de Santiago de Compostela, Rúa Jenaro de la Fuente, s/n, Santiago de Compostela, 15782, SPAIN

²Departamento de Química Física, Universidade de Santiago de Compostela, Facultad de Ciencias, Avda. de Alfonso X o Sabio s/n, Lugo, 27002, SPAIN

E-mail: marcos.rellan@usc.es

Corannulene is an unsaturated polycyclic hydrocarbon, with a central five-membered ring with five six-membered rings around it. Its structure is considered a fragment of C₆₀. Corannulene is a curved π surface, but unlike C₆₀ it has two accessible faces. These faces are quite different: one concave (inside) and one convex (outside). In this work a DFT and MP2 computational study of interaction between corannulene and alkali cations (Li⁺, Na⁺ and K⁺) have been performed. Different isomers of corannulene/M⁺ and transition states, which interconnect them, have been studied. Alkali cations can be pentacoordinated or hexacoordinated to five or six-membered rings of corannulene. This binding can be to both faces. In DFT calculations, binding to the convex face (outside) is favored relative to the concave face for the three alkali. For Li⁺ and Na⁺, MP2 calculations show the same trend, but for K⁺ this trend is reversed. According to our results, migration of cations can be over the convex or concave π -face. To transform a concave complex in a convex complex are two ways: migration across the edge of corannulene and bowl-to-bowl inversion.

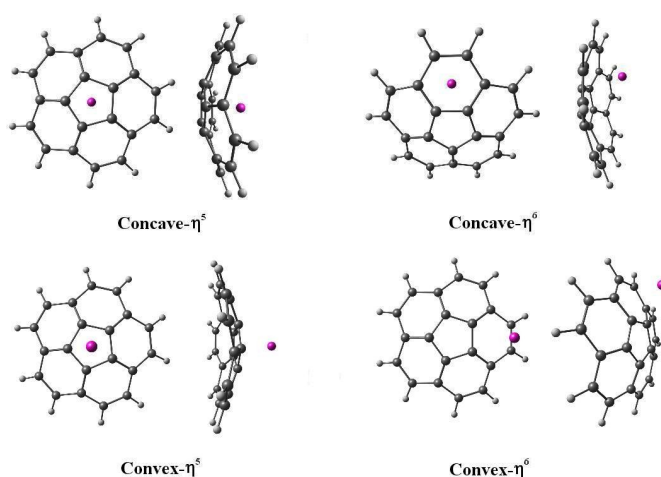


Figure 1.- Geometries of M⁺/corannulene bound to convex and concave sites.

Charge-transfer processes in the assembly of neutral Si_nO_m silicon oxide clusters

Maria Jadraque¹, Margarita Martin¹

¹ Instituto de Química Física “Rocasolano” CSIC, Serrano 119, Madrid 28006, Spain

E-mail: mjadraque@iqfr.csic.es

Experimental and theoretical work have provided evidence for the role of Si_nO_m clusters in the growth of oxide-coated silicon nanowires. It has been proposed that $(\text{SiO})_n$ clusters produced by evaporation of suitable precursors adopt stable structures in which Si_j regions are “segregated” or “cored” by O-rich regions; the latter in turn, are reminiscent of structures containing SiO_2 groups coordinated to $(\text{SiO})_i$ motifs. The thermal decomposition of large $(\text{SiO})_n$ into Si_j and O-rich regions and the different stability of Si-segregated and Si-cored $(\text{SiO})_n$ isomers against oxidation have been studied by *ab initio* molecular dynamics simulations; the different reactivity with oxygen was explained in terms of the electron donor character of $(\text{SiO})_n$ and the degree of accessibility of its reactive sites to the oxygen attack.

Clustering reactions of SiO molecules are also proposed to be at the origin of silica grains and silicates in interstellar environments. Possible routes to the formation of silicates have been investigated. SiO_2 regions can be chemically developed in $(\text{SiO})_i$ motifs or alternatively, formation of silicates could take place by clustering of SiO_2 . Although stable structures have been calculated for several $(\text{SiO}_2)_n$ clusters, the strong oxidant character of SiO_2 for $(\text{SiO})_n$ makes more likely that oxygen-enrichment was the result of $\text{SiO}_2 + (\text{SiO})_n$ reactions.

The prevalence of structures with $(\text{SiO})_n(\text{SiO}_2)_m$ stoichiometry, inferred from the theoretical studies and experimental observations, indicates a strong bonding character between SiO_2 and $(\text{SiO})_n$. In this work, the two lowest terms of the $(\text{SiO})_n(\text{SiO}_2)$ series were taken as model systems to investigate the chemical bonding of these O-rich clusters. To achieve it, the potential energy surfaces (PES) for the aggregation of one SiO_2 molecule to (SiO) and $(\text{SiO})_2$ were calculated, finding evidence for a new reaction route that involves a harpoon-type reaction mechanism.

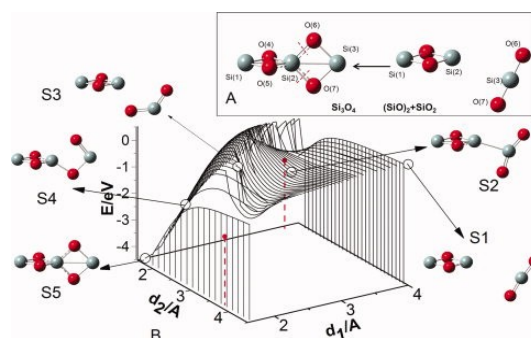


Figure 1: Calculated $(\text{SiO})_2 + \text{SiO}_2 \rightarrow \text{Si}_3\text{O}_4$ PES versus the 2-D reaction coordinate $R(d_{\text{Si}(2)-\text{O}(6)} = d_1, d_{\text{Si}(2)-\text{O}(7)} = d_2)$

Theoretical Bjerrum length of PAH/PSS Polyelectrolyte Bilayers

E.I. Martín¹, A. Sánchez-Coronilla²

¹ *Departamento de Química Física. Universidad de Sevilla*

² *Departamento de Química Física. Facultad de Ciencias. Universidad de Cádiz.*

E-mail: elisamf@us.es

PAH/PSS polyelectrolyte bilayers are commonly formed using Langmuir-Blodgett (LB) deposition or self-assembly techniques based on chemisorption. This method makes use of the electrostatic attraction between oppositely charged polyelectrolytes to produce multilayer thin films. Attending to the internal charge stoichiometry of the polyelectrolytes, some works [1] indicate that the charge stoichiometry of the polyelectrolytes is not 1:1 and it is suggested that if the average distance between the polyelectrolyte charges is less than the Bjerrum length $l_B = e^2/4\pi\epsilon k_B T$ the multilayers contain small counterions which are immobilized on the polyelectrolyte.

In order to clarify the interaction between the polyelectrolytes, a theoretical study on the formation of multilayer films of poly(allylaminehydrochloride) (PAH)/poly(styrene sulphonate) (PSS) is presented (Fig. 1).

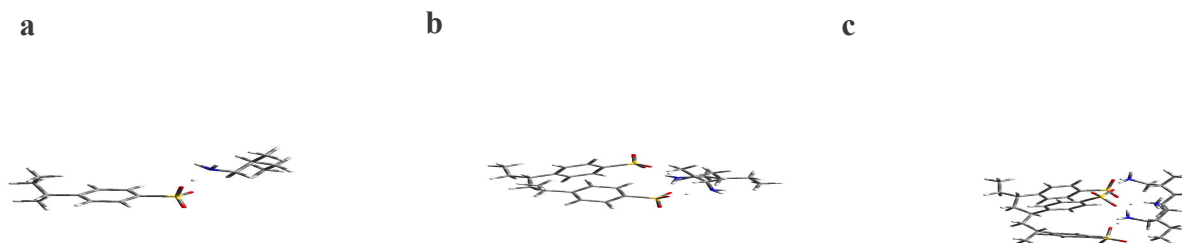


Figure 1: Optimized structure at B3LY/6-31g(d) level for dimeric interaction of a) one PAH/PSS, b) two PAH/PSS and c) three PAH/PSS residues.

[1] H. Riegler, F. Essler, *Langmuir* 18, 6694 (2002).

Haces monoenergéticos de electrones para física fundamental y aplicaciones

J.M. Cornejo, A.M. Lallena and D. Rodríguez

Departamento de Física Atómica Molecular y Nuclear, Universidad de Granada

E-mail: jmcg@ugr.es

Haces monocromáticos de electrones en un rango de energías de 1 - 20 MeV son importantes para realizar medidas de precisión de la función respuesta de detectores de radiación usados en física fundamental, en experimentos de decaimiento β (ver ejemplo [1]), o en aplicaciones, como por ejemplo la determinación del perfil de energía de los electrones de un acelerador clínico. Sin embargo, la producción de estos haces resulta compleja, especialmente si se quiere llevar a cabo con un dispositivo compacto. En la Universidad de Granada (UGR) hemos diseñado y construido un dispositivo basado en un conjunto de electroimanes que presenta importantes características en lo que respecta al sistema de enfriamiento de las bobinas, la calibración del campo magnético y la portabilidad [2]. En esta comunicación, se mostrarán los resultados obtenidos en un primer experimento llevado a cabo en el Centro Nacional de Aceleradores (CNA) en Sevilla (España) usando la reacción $d(7\text{Li}, 8\text{Li})p$, para generar la fuente β [3], y un primer prototipo del dispositivo construido en la UGR. Se mostrarán también las especificaciones técnicas del dispositivo.

[1] X. Fléhard et al, J. Phys. G: Nucl. Part. Phys. 38, 212504 (2011)

[2] J.M. Cornejo, A.M. Lallena and D. Rodríguez, Internal doc for Patent Application (2011)

[3] X. Fléhard et al, Phys. Rev. C 82, 027309 (2010)

Pseudopotentials vs all electron, study applied to solar cells dyes calculations

J. Sánchez Márquez, A. Sánchez-Coronilla, D. Zorrilla, J. Navas, R. Alcántara, C. Fernandez-Lorenzo and J.M. Calleja

¹ *Departamento de Química Física.
Universidad de Cádiz. Facultad de Ciencias. Apartado 11510 Puerto Real (Cádiz).*

E-mail: jesus.sanchezmarquez@uca.es

Dye-Sensitized solar cells (DSSCs) are one of the emerging solar technologies that offer the potential to reduce the cost of photovoltaic electricity generation [1]. Over last 20 years there has been extensive academic and, increasingly, commercial interest in this technology.

The primary energy conversion process in dye-sensitized solar cells is a photoinduced charge separation at the metal oxide/dye/electrolyte interface. We focus upon considering how advances in fundamental understanding can help guide materials and device development.

In reference [2] pseudopotential results and all electron ones were too different. In our work we have compared pseudopotentials vs all electron basis-set and we have focused on molecular geometry and some electronic properties. We have tested several Method/Pseudopotential/basis-set in order to find the best combinations and we have used well known simple molecules to compare with the experimental data.

[1] Andrea Listorti, Brian O'Regan and James R Durrant, Chem. Mater, 23, 3381–3399 (2011).

[2] Frederick P. Arnold, Jr, Organometallics, 18, 4800-4809 (1999).

Study of the critical solutions of Dyson-Schwinger equations at infrared region.

Adrian Ayala-Gomez¹, Jose Rodriguez-Quintero¹

¹*Faculty of Experimental Sciences, University of Huelva. Avenida de las Fuerzas Armadas s/n.
21071. Huelva.Spain*

E-mail:jose.rodriguez@dfaie.uhu.es

The problem of quarks confinement is one of the most compelling in QCD. The study of Green functions of the theory at low momentum region is thought to shed light on the mechanism of confinement. In this communication we calculate the form factor of the ghost propagator (one of QCD Green functions), solving ghost propagator Dyson-Schwinger equations (DSE) at low momentum (infrared region). Even though there are two families of solutions (scaling and decoupling, scaling one being singular at 0 momentum), both, numerical solutions of DSE and lattice simulations, show that the scaling solution is physically meaningless. Contrarely, decoupling solutions are found, which implies finite ghost and a non-vanishing gluon propagator at $k = 0$ momentum. We solve DSE for different numbers of quark flavours (N_f), and find emergence of critical behaviour (scaling solutions) only for a certain value of coupling constant (α). An improvement of ghost propagator, with a refined expresion of ghost-gluon vertex (calculated using OPE technique), is also accomplished.

Theoretical study of the pyridine–(helium) $_n$, $n = 1, 2$, van der Waals complexes

Hubert Cybulski¹, Berta Fernández¹, Antonio Gamboa², Rosa M. Benito², Angeline Wairegi², David Farrelly²

¹*Department of Physical Chemistry and Center for Research
in Biological Chemistry and Molecular Materials (CIQUS)
University of Santiago de Compostela
E-15782 Santiago de Compostela, Spain*

²*Department of Chemistry and Biochemistry
Utah State University, Logan
UT 84322-0300, USA
E-mail: hcybulski@gmail.com*

The high-level *ab initio* theoretical studies for the ground-state intermolecular potential-energy surfaces (IPESs) of the pyridine–(helium) $_n$ ($n = 1, 2$) complexes are being carried out. The interaction energy calculations are performed with the CCSD(T) method and the aug-cc-pVDZ-33211 basis set. The surface minima for the pyridine–helium system are characterized by the He atom located above and below the pyridine ring. To shed more light into the nature of the intermolecular interactions, we use the symmetry-adapted perturbation-theory (SAPT). For the larger complex different isomers resulting from binding helium atoms to the same side of the aromatic ring plane or to both sides are considered. In this system, the influence of three-body effects is also estimated.

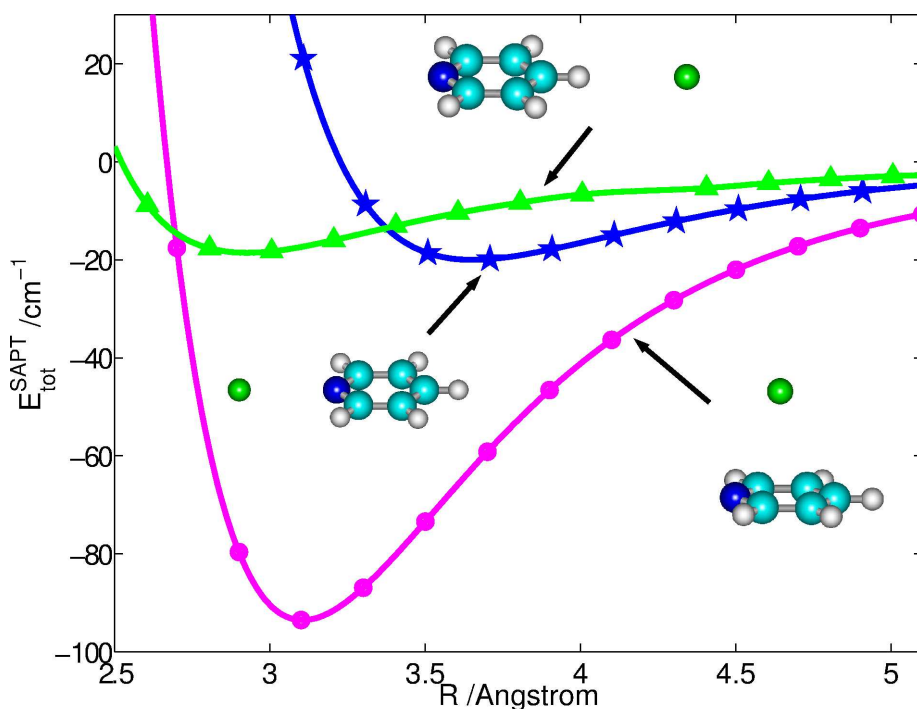


Figure 1: The total SAPT interaction energy for the pyridine–helium complex

List of Participants

Acosta Gutiérrez, Silvia
silviaa.gutierrez@gmail.com
Universidad de La Laguna
Tenerife

Ayala Gómez, Adrián
adrayala03@hotmail.com
Universidad de Huelva
Huelva

Balerdi Villanueva, Garikoitz
garikoitz.bv@gmail.com
Universidad Complutense de Madrid
Madrid

Bouvrie, Peter Alexander
bouvrie@ugr.es
Universidad de Granada
Granada

Campo Cacharrón, Alba
alba.campoca@gmail.com
Universidade de Santiago de Compostela
Santiago de Compostela

Corrales Castellanos, María Eugenia
me.corrales@quim.ucm.es
Universidad Complutense de Madrid
Madrid

Cornejo García, Juan Manuel
jmcg@ugr.es
Universidad de Granada
Granada

Cybulski, Hubert
hcybulski@gmail.com
Universidade de Santiago de Compostela
Santiago de Compostela

García Ferreira, Ix-Berenice
ixbgf@ugr.es
Universidad de Granada
Granada

González Infantes, Wilfredo
wgonzalez@ugr.es
Universidad de Granada
Granada

González González, Marta
marta.glezglez@hotmail.com
Universidad Complutense de Madrid
Madrid

Guerrero Martínez, Ángel
agmartinez@ugr.es
Universidad de Granada
Granada

Heimsoth, Martin
heimsoth@fis.ucm.es
Universidad Complutense de Madrid
Madrid

Jadraque, María
mjadraque@iqfr.csic.es
Instituto de Física-Química Rocasolano” (CSIC)
Madrid

López Rosa, Sheila
slopez@ugr.es
Universidad de Sevilla
Sevilla

Majtey, Ana
anamajtey@ugr.es Universidad de Granada
Granada

Martín Fernández, Elisa Isabel
elisamf@us.es
Universidad de Sevilla
Sevilla

Navarro Pérez, Rodrigo
rnavarro@ugr.es
Universidad de Granada
Granada

Nogueira Pérez, Juan José
juanjonog@hotmail.com
Universidade de Santiago de Compostela
Santiago de Compostela

Omiste Romero, Juan José
omiste@ugr.es
Universidad de Granada
Granada

Rellán Piñeiro, Marcos
marcosrellan@hotmail.com
Universidade de Santiago de Compostela
Santiago de Compostela

Rodríguez Díaz, Javier
javier.rodriguez.diaz@quim.ucm.es
Universidad Complutense de Madrid
Madrid

Ruiz Simó, Ignacio Luis
igruizsi@ific.uv.es
Universidad de Granada
Granada

Sánchez Coronilla, Antonio
antonio.coronilla@uca.es
Universidad de Cádiz
Cádiz

Sánchez Márquez, Jesús
jesus.sanchezmarquez@uca.es
Universidad de Cádiz
Cádiz