Departamento de Química

FACULTAD DE CIENCIAS
UNIVERSIDAD AUTÓNOMA DE MADRID

DEPARTAMENTO DE QUÍMICA
MEMORIA DE INVESTIGACIÓN
2017

UAM
UNIVERSIDAD AUTONOMA
DE MADRID

MEMORIA DE INVESTIGACIÓN DEL DEPARTAMENTO DE QUÍMICA 2017

	ARTICULOS	OTRAS PUBLICACIONES
BIOLOGIA	**124**	**9**
BIOLOGIA MOLECULAR	**100**	**11**
ECOLOGIA	**62**	**5**
FISICA APLICADA	**25**	**7**
FISICA DE MATERIALES	**26**	**7**
FISICA DE LA MATERIA CONDENSADA	**68**	**2**
FISICA TEORICA	**172**	**12**
FISICA TEORICA DE LA MATERIA CONDENSADA	**38**	**3**
GEOLOGIA	**36**	**10**
MATEMATICAS	**85**	**6**
QUIMICA	**58**	**6**
QUIMICA AGRICOLA	**23**	**2**
QUIMICA ANALITICA	**9**	**2**
QUIMICA FISICA APLICADA	**111**	**2**
QUIMICA INORGANICA	**21**	**1**
QUIMICA ORGANICA	**44**	**3**
FACULTAD DE CIENCIAS	**942**	**79**

PUBLICACIONES EN 2017 (58)

Aguilar-Galindo, F; Ocón, P; López Poyato, J.M. Exploring the catalytic efficiency of X-doped (X=B, N, P) graphene in oxygen reduction reaction: Influence of solvent and border effects. INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY
http://www.onlinelibrary.wiley.com/doi/10.1002/qua.25579/abstract

Aguirre N; Diaz-Tendero S; Hervieux P; Alcami M; Martín F (2017). M_3C: A Computational Approach to Describe Statistical Fragmentation of Excited Molecules and Clusters. JOURNAL OF CHEMICAL THEORY AND COMPUTATION, 13(3), 992-1009. DOI: 10.1021/acs.jctc.6b00984

Alkorta I; Montero-Campillo M; Elguero J (2017). Trapping CO_2 by Adduct Formation with Nitrogen Heterocyclic Carbenes (NHCs): A Theoretical Study. CHEMISTRY - A EUROPEAN JOURNAL, 23(44), 10604-10609. DOI: 10.1002/chem.201701444

Argenti L; Jiménez-Galán; Caillat J; Taïeb R; Maquet A; Martín F (2017). Control of photoemission delay in resonant two-photon transitions. PHYSICAL REVIEW A - ATOMIC, MOLECULAR, AND OPTICAL PHYSICS, 95(4).DOI: 10.1103/PhysRevA.95.043426

Arpa, EM; Aguilar-Galindo, F; Diaz-Tendero, S (2017). Unravelling the Mechanism of Non-photoactivated [2+2] Cycloaddition Reactions: Relevance of Orbital Interactions and Zwitterionic Intermediates. CHEMISTRY SELECT, 2(3), 1089-1093. DOI: 10.1002/slct.201601743

Arslancan S; Martínez-Fernández L; Corral I (2017). Photophysics and photochemistry of canonical nucleobases' thioanalogs: From quantum mechanical studies to time resolved experiments. MOLECULES, 22(6).DOI: 10.3390/molecules22060998

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Barandiarán, Z; Betinelli, M; Seijo, L. Color control of Pr^{3+} luminescence by electron-hole recombination energy transfer in $CaTiO_3$ and $CaZrO_3$. Journal of Physical Chemistry Letters, **8** (2017) 3095-3100.

Bolognesi, P; Bañares, L; Alcamí, M. XUV/X-ray light and fast ions for ultrafast chemistry PHYSICAL CHEMISTRY CHEMICAL PHYSICS 19, 19533-19535 (2017)

Bruña, Sonia; González-Vadillo, Ana M.; Ferrández, Marta; Perles, Josefina; Montero-Campillo, M. Merced; Mó, Otilia; Cuadrado, Isabel. Formation of unexpected silicon- and disiloxane-bridged multiferrocenyl derivatives bearing Si-O-CHCH2 and Si-(CH2)2C(CH3)3 substituents via cleavage of tetrohydrofuran and trapping of its ring fragments. Dalton Transactions 2017, 46, 11584-11597, DOI: 10.1039/C7DT02286G.

Chicharro D; Marggi Poullain S; González-Vazquez J; Bañares L (2017). Slice imaging of the UV photodissociation of CH_2BrCl from the maximum of the first absorption band. JOURNAL OF CHEMICAL PHYSICS, 147(1), 013945-. DOI: 10.1063/1.4984789

Corral I; González-Vazquez J; Martín F (2017). Potential Energy Surfaces of Core-Hole and Shake-Up States for Dissociative Ionization Studies. JOURNAL OF CHEMICAL THEORY AND COMPUTATION, 13(4), 1723-1736. DOI: 10.1021/acs.jctc.6b01214

Cueto, Marcos del; Muzas, Alberto A; Somers, Mark F.; Kroes, Geert-Jan; Diaz, Cristina; Martín; Fernando (2017). Exploring surface landscapes with molecules: rotationally induced diffraction of H2 on LiF(001) under fast grazing incidence conditions. PHYSICAL CHEMISTRY CHEMICAL PHYSICS, 19(25), 16317-16322. DOI: 10.1039/c7cp02904g

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Diaz-Tendero, S; Piekarski, DG; (2017). Structure and stability of clusters of beta-alanine in the gas phase: importance of the nature of intermolecular interactions. PHYSICAL CHEMISTRY CHEMICAL PHYSICS, 19(7), 5465-5476. DOI: 10.1039/c6cp07792g

García-Rodríguez D; Mendoza-Huizar L; Diaz C (2017). A DFT study of Cu nanoparticles adsorbed on defective graphene. APPLIED SURFACE SCIENCE, 412, 146-151. DOI: 10.1016/j.apsusc.2017.03.239

Gómez C; Pisarra M; Gravina M; Sindona A (2017). Tunable plasmons in regular planar arrays of graphene nanoribbons with armchair and zigzag-shaped edges. BEILSTEIN J NANOTECH, 8(1), 172-182. DOI: 10.3762/bjnano.8.18

Gomez CV; Pisarra M; Gravina M; Riccardi P, Sindona A (2017). Plasmon properties and hybridization effects in silicene. PHYSICAL REVIEW B 95(8), 085419. DOI: 10.1103/PhysRevB.95.085419

Grossi J, Kooi DP, Giesbertz KJH, Seidl M, Cohen AJ, Mori-Sánchez P, Gori-Giorgi P (2017). Fermionic Statistics in the Strongly Correlated Limit of Density Functional Theory.. JOURNAL OF CHEMICAL THEORY AND COMPUTATION, 13(12), 6089-6100. DOI: 10.1021/acs.jctc.7b00998

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Jelovina D; Feist J; Martín F; Palacios A (2017). Imaging ultrafast molecular wave packets with a single chirped UV pulse. PHYSICAL REVIEW A - ATOMIC, MOLECULAR, AND OPTICAL PHYSICS, 95(4), ARTN 043424-. DOI: 10.1103/PhysRevA.95.043424

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Lara-Astiaso M; Palacios A; Decleva P; Tavernelli I; Martín F (2017). Role of electron-nuclear coupled dynamics on charge migration induced by attosecond pulses in glycine. CHEMICAL PHYSICS LETTERS, 683, 357-364. DOI: 10.1016/j.cplett.2017.05.008

Ligny, R; Yáñez, M; Roisnel, T; Guillemin, J-C; Trolez, Y (2017). One-step synthesis of conjugated enynenitriles from bromocyanoacetylene. Org. Biomol. Chem. **15**, 6050-6056 (2).

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Marggi Poullain S; Chicharro D; González-Vazquez J; Rubio-Lago L; Bañares L (2017). A velocity map imaging study of the photodissociation of the methyl iodide cation. PHYSICAL CHEMISTRY CHEMICAL PHYSICS, 19(11), 7886-7896. DOI: 10.1039/c7cp00319f

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Montero-Campillo M; Corral I; Mo O; Yanez M; Alkorta I; Elguero J (2017). Beryllium-based fluorenes as efficient anion sponges. PHYSICAL CHEMISTRY CHEMICAL PHYSICS, 19(34), 23052-23059. DOI: 10.1039/c7cp03664g

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Revuelta F; Vergini E; Benito R; Borondo F (2017). Semiclassical basis sets for the computation of molecular vibrational states. JOURNAL OF CHEMICAL PHYSICS, 146(1).DOI: 10.1063/1.4973376

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Sturm F; Tong X; Palacios A; Wright T; Zalyubovskaya I; Ray D; Shivaram N; Martín F; Belkacem A; Ranitovic P; Weber T (2017). Mapping and controlling ultrafast dynamics of highly excited H2 molecules by VUV-IR pump-probe schemes. PHYSICAL REVIEW A - ATOMIC, MOLECULAR, AND OPTICAL PHYSICS, 95(1), ARTN 012501-. DOI: 10.1103/PhysRevA.95.012501

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Wang Y; Diaz-Tendero S; Alcami M; Martín F (2017). Relative stability of empty exohedral fullerenes: Π Delocalization versus strain and steric hindrance. JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 139(4), 1609-1617. DOI: 10.1021/jacs.6b11669

Wang, Y; Diaz-Tendero, S; Alcami, M; Martin F. (2017). Generalized structural motif model for studying the thermodynamic stability of fullerenes: from C-60 to graphene passing through giant fullerenes. PHYSICAL CHEMISTRY CHEMICAL PHYSICS, 19 (30), 19646-19655. DOI: 10.1039/c7cp01598d

OTRAS PUBLICACIONES (6)

En esta sección incluimos capítulos de libros, conferencias publicadas, editoriales, erratum, meeting-abstract y short survey

Meeting-Abstract

Argenti L, Jiménez Galán A, Taïeb R, Caillat J, Maquet A, Martín F (2017). Control of photoemission delay in resonant two-photon transitions. JOURNAL OF PHYSICS: CONFERENCE SERIES, 875(3), -. DOI: 10.1088/1742-6596/875/3/022040

Erdmann E, ?abuda M, Diaz-Tendero S, Aguirre N, Alcami M (2017). Charge dependence of fragmentation process induced by ion collisions with furan molecule. JOURNAL OF PHYSICS: CONFERENCE SERIES, 875(11), -. DOI: 10.1088/1742-6596/875/11/102021

Mahajan T, Id Barkach T, Aguirre N, Alcami M, Bonnin M, Chabot M, Diaz-Tendero S, Geslin F, Hamelin T, Hammache F, Illescas C, Jallat A, Jorge A, Launoy T, Le T, Lepadellec A, Martín F, Meyer A, Perrot L, Pino T, Pons B, De Séréville N, Béroff K (2017). Excitation and fragmentation in high velocity C_nN^+- He collisions. JOURNAL OF PHYSICS: CONFERENCE SERIES, 875(11), -. DOI: 10.1088/1742-6596/875/11/102022

Rabadán I, Méndez L (2017). Orientation effects in ion-molecule collisions. JOURNAL OF PHYSICS: CONFERENCE SERIES, 875(2), -. DOI: 10.1088/1742-6596/875/2/012009

PROYECTOS DE INVESTIGACIÓN ACTIVOS EN 2017

CALCULO DE DATOS ATOMICOS Y MOLECULARES FUNDAMENTALES PARA LA MODELIZACION DEL BORDE DEL PLASMA EN ITER
A desarrollar entre: 01/01/2015 y 31/10/2018
Referencia: ENE2014-52432-R
Investigadores UAM: MENDEZ AMBROSIO, LUIS
Departamento: QUÍMICA

IMAGING-XCHEM: A COMPUTATIONAL PACKAGE FOR ULTRAFAST ELECTRONIC CONTROL OF CHEMISTRY
A desarrollar entre: 01/11/2017 y 30/04/2019
Referencia: 780284
Investigadores UAM: Fernando Martín García
Departamento: QUÍMICA

LUMINISCENCIA Y TRANSFERENCIA DE ENERGIA EN MATERIALES FOSFORESCENTES Y DE

CENTELLEO CO LANTANIDOS, UTILES EN ILUMINACION E IMAGENES MEDICAS. ESTUDIOS AB INITIO
A desarrollar entre: 01/01/2015 y 31/12/2017
Referencia: MAT2014-54395-P
Investigadores UAM: BARANDIARAN PIEDRA, ZOILA
Departamento: QUÍMICA

MATERIALES AVANZADOS DE CARBONO PARA FOTOVOLTAICA MOLECULAR
A desarrollar entre: 01/10/2014 y 30/09/2018
Referencia: S2013/MIT-2841
Investigadores UAM: YAÑEZ MONTERO, MANUEL
Departamento: QUÍMICA

MODIFICACION DE LA REACTIVIDAD Y DISEÑO DE NUEVOS MATERIALES MEDIANTE ENLACES BERILIO Y OTRAS INTERACCIONES NO-COVALENTES
A desarrollar entre: 01/01/2016 y 30/09/2019
Referencia: CTQ2015-63997-C2-1-P
Investigadores UAM: YAÑEZ MONTERO, MANUEL
Departamento: QUÍMICA

SISTEMAS MOLECULARES COMPLEJOS EN CONDICIONES ATIPICAS: IONIZACION Y EXCITACION DE MOLECULAS, AGREGADOS Y MATERIALES HIBRIDOS
A desarrollar entre: 30/12/2016 y 29/12/2019
Referencia: CTQ2016-76061-P
Investigadores UAM: ALCAMI PERTEJO, MANUEL; DIAZ-TENDERO VICTORIA, SERGIO
Departamento: QUÍMICA

SOLICITUD DE UN PROYECTO ITN-JD EN QUÍMICA TEORICA ORIENTADA AL DISEÑO MOLECULAR
A desarrollar entre: 01/07/2017 y 31/12/2018
Referencia: EUIN2017-87323
Investigadores UAM: ALCAMI PERTEJO, MANUEL
Departamento: QUÍMICA

STABILITY AND TRANSITIONS IN PHYSICAL PROCESSES - TraX
A desarrollar entre: 01/03/2017 y 28/02/2021
Referencia: GA 734557
Investigadores UAM: Florentino Borondo Rodriguez
Departamento: QUÍMICA

EUROPEAN JOINT DOCTORTATE "THEORETICAL CHEMISTRY AND COMUTATIONAL MODELLING – TCCM"
A desarrollar entre: 01/01/2015 y 31/12/2018
Referencia: GA 642294
Investigadores UAM: Manuel Yáñez Montero
Departamento: QUÍMICA

ERAMUS+ MASTER "THEORETICAL CHEMISTRY AND COMPUTATIONAL MODELLING

A desarrollar entre: 4 ediciones bi-anuales (01/09/2015 a 31/08/2019)
Referencia: TCCM
Investigadores UAM: Manuel Yáñez Montero
Departamento: QUÍMICA

ULTRAHIGH PRESSURE CHEMISTRY AT THE NANOSCALE

A desarrollar entre: 01/01/2017 y 30/06/2019
Referencia: Proyectos colaborativos de investigación (2016)
Investigadores UAM: Fernando Martín García
Departamento: QUÍMICA

COMPUTACIÓN EN CIENCIA DE ATTOSEGUNDOS Y DE MATERIALES: AFRONTANDO LOS NUEVOS RETOS DE LA FÍSICA Y LA QUÍMICA ACTUALES

A desarrollar entre: 30/12/2016 y 29/12/2019
Referencia: FIS2016-77889-R
Investigadores UAM: Fernando Martín García
Departamento: QUÍMICA

MATERIALES METAL-ORGÁNICOS BIOINSPIRADOS E INTELIGENTES CON COMPORTAMIENTO ESTÍMULO-RESPUESTA

A desarrollar entre: 01/01/2017 y 31/12/2019
Referencia: MAT2016-75883-C2-2-P
Investigadores UAM: Mª Luisa Marcos Laguna
Departamento: QUÍMICA

RED TEMÁTICA SOBRE "DINÁMICA, TRACTORES, NO LINEALIDAD. CAOS Y ESTABILIDAD"
A desarrollar entre: 01/03/2017 al 28/02/2019
Referencia: MTM2016-81902-REDT
Investigadores UAM: Florentino Borondo Rodríguez
Departamento: QUÍMICA

CAOS CUÁNTICO Y CLÁSICO EN SISTEMAS DINÁMICOS Y COMPLEJIDAD
A desarrollar entre: 01/01/2016 a 31/12/2018
Referencia: MTM2015-63914-P
Investigadores UAM: Florentino Borondo Rodríguez
Departamento: QUÍMICA

DOTACIÓN ADICIONAL RAMÓN Y CAJAL
A desarrollar entre: 2011-2017
Referencia: RYC-2011-07019
Investigadores UAM: Sergio Díaz Tendero Victoria
Departamento: QUÍMICA

DOTACIÓN ADICIONAL RAMÓN Y CAJAL
A desarrollar entre: 2014-2018
Referencia: RYC-2013-14586
Investigadores UAM: Cristina Díaz Blanco
Departamento: QUÍMICA

DOTACIÓN ADICIONAL RAMÓN Y CAJAL
A desarrollar entre: 01/11/2015 al 31/10/2019
Referencia: RYC-2014-16706
Investigadores UAM: Alicia Palacios Cañas
Departamento: QUÍMICA

DOTACIÓN ADICIONAL JUAN DE LA CIERVA
A desarrollar entre: 01/02/2017 al 31/01/2019
Referencia: IJCI-2015-26997
Investigadores UAM: Etienne Plesiat
Departamento: QUÍMICA

NUEVAS FRONTERAS DEL NANOMAGNETISMO FUNDAMENTAL Y APLICADO (NANOFRONTMAG-CM)

A desarrollar entre: 01/10/2014 a 31/12/2018
Referencia: S2013/MIT-2850
Investigadores UAM: Fernando Martín García
Departamento: QUÍMICA

COMPUTACIÓN EN CIENCIA DE ATTOSEGUNDOS Y DE MATERIALES
A desarrollar entre: 01/03/2017 a 28/02/2019
Referencia: PEJD-2016/IND-3217
Investigadores UAM: Fernando Martín García
Departamento: QUÍMICA

AYUDAS PARA LA ATRACCIÓN DE TALENTO INVESTIGADOR 2016 - CATEGORÍA 2

A desarrollar entre: 01/03/2017 a 28/02/2021
Referencia: 2016-T2/IND-1660
Investigadores UAM: Ana Martín Sómer
Departamento: QUÍMICA

XUV/X-RAY LASERS FOR ULTRAFAST ELECTRONIC CONTROL IN CHEMISTRY (XCHEM)

A desarrollar entre: 01/01/2012 a 31/08/2017
Referencia: ERC-AdG-2011-GA 290853-XCHEM
Investigadores UAM: Fernando Martín García
Departamento: QUÍMICA

XUV/X-RAY LIGHT AND FAST IONS FOR ULTRAFAST CHEMISTRY (XLIC)
A desarrollar entre: : 13/05/2013 a 12/05/2017
Referencia: COST Action CM1204
Investigadores UAM: Fernando Martín García
Departamento: QUÍMICA

TESIS DOCTORALES DEL DEPARTAMENTO QUÍMICA EN 2017 (8)

Programas de Doctorado regulados por el RD 1393/2007

Doctorado en Química Teórica y Modelización Computacional (5)

FRAGMENTATION DYNAMICS OF IONISED AMINO ACIDS AND NEUTRAL CLUSTERS OF AMINO ACIDS IN THE GAS PHASE: A THEORETICAL STUDY

Autor: Piekarski, Dariusz Grzegorz

Director/es: Alcami Pertejo, Manuel y Díaz-Tendero Victoria, Sergio

Tutor: Mo Romero, Otilia

Desarrollada en: Departamento de Química

NOVEL TOOLS FOR THE ANALYSIS OF NON-STANDARD CHEMICAL BONDS: THEORETICAL INSIGHT INTO THE NATURE OF BERYLLIUM BONDS

Autor: Brea Noriega, Oriana

Director/es: Yañez Montero, Manuel y Corral Pérez, Ines

Tutor: Yañez Montero, Manuel

Desarrollada en: Departamento de Química

PHOTOIONIZATION OF STRONGLY CORRELATED MANY-ELECTRON ATOMS AND MOLECULES: A HYBRID-BASIS CLOSE-COUPLING INTERFACE TO QUANTUM CHEMISTRY PACKAGES

Autor: Marante Valdés, Carlos Antonio

Director/es: Argenti, Luca y Martín García, Fernando

Tutor: Martín García, Fernando

Desarrollada en: Departamento de Química

THEORETICAL TREATMENT OF INELASTIC PROCESSES IN ATOMIC COLLISIONS INVOLVING ONE AND MANY ELECTRON SYSTEMS

Autor: Jorge Palacios, Alba María

Director/es: Illescas Rojas, Clara Matilde

Tutor: Illescas Rojas, Clara Matilde

Desarrollada en: Departamento de Química

ULTRAFAST PROCESSES IN N2 PHOTOIONIZATION: IMPLEMENTACION OF THE XCHEM CODE

Autor: Klinker, Markus

Director/es: González Vázquez, Jesús y Martín García, Fernando

Tutor: González Vázquez, Jesús

Desarrollada en: Departamento de Química

Programas de Doctorado regulados por el RD 99/2011

Programa de Doctorado en Química Teórica y Modelización Computacional (3)

A FULL DIMENSIONAL DISCRETE VARIABLE REPRESENTATION OF H+ 2 AND H2 PHOTOIONIZATION

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Director/es: Palacios Cañas, Alicia y Martín García, Fernando

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Desarrollada en: Departamento de Química

IMAGING ULTRAFAST ELECTRON AND NUCLEAR DYNAMICS IN HYDROGENIC MOLECULES

Autor: Bello Romero, Roger Yulier

Director/es: Palacios Cañas, Alicia y Martín García, Fernando

Tutor: Palacios Cañas, Alicia

Desarrollada en: Departamento de Química

SIMULATIONS OF AQUEOUS SYSTEMS: FROM GAS TO THE CONDENSED PHASE

Autor: Arismendi Arrieta, Daniel José

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Tutor: Alcami Pertejo, Manuel

Desarrollada en: Consejo Superior de Investigaciones Científicas-Instituto de Física