PERSONAL DATA

Family Name SODUPE ROURE
Forename Mariona

ID/Passport no 46118937-G
Date of birth 10/04/1962
Gender: Female
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PRESENT POSITION

Full Professor of Physical Chemistry

Departament de Química, Universidad Autónoma de Barcelona
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ACADEMIC BACKGROUND

- Graduate in Chemistry, (UAB), Universidad Autónoma de Barcelona, June 1985
- Master on Theoretical Chemistry, Universidad Autónoma de Barcelona, 1987
- PhD in Chemistry, Universidad Autónoma de Barcelona, (UAB), April 1990
  (Thesis Supervisors: Jose Maria Lluch and Antoni Oliva)

PAST POSITIONS AND SCIENTIFIC EXPERIENCE

- 1986-1988 Predoctoral research fellow, Department of Chemistry UAB
- 1988-1990 Teaching assistant at the Department of Chemistry UAB.
- 1990-1992 Postdoctoral Fulbright fellow at NASA Ames Reseach Center (California).
- 1992-1996 Temporary Associate Professor, Department of Chemistry UAB
- 1996-2008 Associate Professor, Department of Chemistry UAB
- 2008- present Full Professor, Department of Chemistry UAB.

RESEARCH INTERESTS

Main research interests focus on the structure and reactivity of bioinorganic systems using quantum chemical methods. Recent projects focus on the computational modelling of i) complex metal cation-biomolecule systems, with special focus on their role in neurodegenerative

diseases, and iii) the adsorption and reactivity of biomolecules on silica based surfaces, in the context of prebiotic chemistry.

AWARDS

- Special Bachelor's Award "Premio extraordinario de licenciatura", 1985
- Special PhD Award "Premio extraordinario de doctorado", 1990
- Distinction of the Generalitat of Catalunya for the promotion of the research at the University. Category: Young Investigator, June 2001
- ICREA Acacademia 2011

PROFESIONAL ACTIVITIES

Scientific Committees

- Spanish National Plan for Research and Development: Member of the management team of the Chemistry area. (2008-2012)
- Member of the Commission for the accreditation of the Collaborating and Tenure-Track Lecturer in the Catalan University Quality Assurance Agency (AQU) (2008-Present)
- Barcelona Supercomputing Center (BSC): Coordinator of the project selection committee on Chemistry and Material Science Areas (2007-2012)
- Reviewer of research projects for Junta de Andalucía, Agencia Andaluza de Evaluación (AGAE), Xunta de Galicia and Gobierno de Aragón (2005-2009)

Editorial Board membership

- Guest Editor of the Special Issue "Theoretical Chemistry in Spain" of the Journal Theoretical Chemistry Accounts 2010.

Administration

- Director of the Chemical Physics area, University Autónoma Barcelona, 2000-2002
- Coordinator of the Spanish interuniversity master Theoretical and Computational Chemistry, 2003-2005
- Member of the management team of the Chemistry Department, Research area, 2004-2007
- Coordinator for the implementation of the new curricula of chemistry at the Universidad Autónoma de Barcelona, 2009-2010
- Member of the steering committee of the Reference Network of Theoretical and Computational Chemistry, (2006- 2012)

Stays in foreign centres (more than one month)

Postdoctoral stay: NASA Ames Research Center, Moffet Field (California) 2 years (1990-92)

PARTICIPATION IN RESEARCH PROJECTS

1. PROJECT TITLE: "Reacciones de las especies radicalarias cargadas en clusters con enlaces de hidrógeno y en procesos de transferencia electrónica disociativa"
   FUNDING AGENCY: DGICYT PB89-0318
   LENGTH FROM: 1990 TO: 1993
   PRINCIPAL INVESTIGATOR: Juan Bertrán

2. PROJECT TITLE: Grupo de Química Teórica
   FUNDING AGENCY: CIRIT, Grups de recerca de qualitat GRQ 93-2079
   LENGTH FROM: 1993 TO: 1995
   PRINCIPAL INVESTIGATOR: Antonio Oliva

3. PROJECT TITLE: "Estructura y reactividad de complejos de metales de transición. Interacción metal-ligando y activación molecular"
   FUNDING AGENCY: DGICYT PB92-0621
   BUDGET: 14.000.000
   LENGTH FROM: 1993 TO: 1996
   PRINCIPAL INVESTIGATOR: Antonio Oliva

4. PROJECT TITLE: Grupo de Química Teórica
   FUNDING AGENCY: DGR 1995 SGR-00401
   LENGTH FROM: 1996 TO: 1997
   PRINCIPAL INVESTIGATOR: Antonio Oliva

5. PROJECT TITLE: "Estructura y reactividad de complejos metálicos. Aplicaciones en síntesis orgánica y en química ambiental"
   FUNDING AGENCY: DGESIC PB95-0640
   BUDGET: 7.000.000 pts
   LENGTH FROM: 1996 TO:1999
   PRINCIPAL INVESTIGATOR: Antonio Oliva

6. PROJECT TITLE: Grupo de Química Teórica
   FUNDING AGENCY: DGR, 1997 SGR-0004
   LENGTH FROM: 1997 TO: 1999
   BUDGET: 1.350.000 pts
   PRINCIPAL INVESTIGATOR: Antonio Oliva

7. PROJECT TITLE: "Estructura y reactividad de complejos metálicos. Aplicaciones en Química ambiental y en sistemas de interés bioquímico"
   FUNDING AGENCY: DGESIC PB98-0912
   LENGTH FROM: 1999 TO: 2002
   BUDGET: 10.500.000 pts
   PRINCIPAL INVESTIGATOR: Antonio Oliva

8. PROJECT TITLE: Grupo de estructura y reactividad Química

FUNDING AGENCY: DGR, 1999 SGR-00092
LENGTH FROM: 1999 TO: 2001
BUDGET: 3.100.000 pts
PRINCIPAL INVESTIGATOR: Antonio Oliva

9. PROJECT TITLE: Grupo de estructura y reactividad Química
FUNDING AGENCY: DGR, 2001 SGR-00182
LENGTH FROM: 2001 TO: 2004
BUDGET: 7.000.000 pts
PRINCIPAL INVESTIGATOR: Juan Bertran

10. PROJECT TITLE: Cationización e ionización de aminoácidos y péptidos
FUNDING AGENCY: DURSI Programa de Distinción de la Generalitat de Catalunya para la promoción de la investigación universitaria
LENGTH FROM: 2001 TO: 2005
BUDGET: 20.000.000 pts
PRINCIPAL INVESTIGATOR: M. Sodupe

11. PROJECT TITLE: Ionización y activación por cationes metálicos de sistemas de interés bioquímico. Estudios teóricos y de espectrometría de masas
FUNDING AGENCY: MCyT (Proyecto coordinado BQU2002-04112-C02-01)
LENGTH FROM: 2003 TO: 2005
BUDGET: 114825 €
PRINCIPAL INVESTIGATOR: M. Sodupe

12. PROJECT TITLE: Activación de biomoléculas. Estudios computacionales y de espectrometria de masas
FUNDING AGENCY: MEC (CTQ2005-08797-C02-02/)
LENGTH FROM: 2006 TO: 2008
BUDGET: 85680 €
PRINCIPAL INVESTIGATOR: M. Sodupe

13. PROJECT TITLE: Grup d'Estudis teòrics d'activació de biomolècules
FUNDING AGENCY: DURSI 2005-SGR-00244
LENGTH FROM: 2005 TO: 2008
BUDGET: 41200 €
PRINCIPAL INVESTIGATOR: M. Sodupe

14. PROJECT TITLE: Researcher's Night
FUNDING AGENCY: FP7-PEOPLE-NIGHT (No 228736). (Funding for Dissemination of Science)
LENGTH FROM: 2008 TO: 2008
BUDGET: 12189 €
PRINCIPAL INVESTIGATOR: M. Sodupe

15. PROJECT TITLE: Activación de biomoléculas por cationes metálicos y superficies siliceas
FUNDING AGENCY: MICINN CTQ2008-06381/BQU
LENGTH FROM: 2009 TO: 2011
BUDGET: 149314 €
PRINCIPAL INVESTIGATOR: M. Sodupe

16. PROJECT TITLE: Grup d'Estudis teòrics d'activació de biomolècules
FUNDING AGENCY: DURSI 2008-SGR-00638
LENGTH FROM: 2009 TO: 2013
BUDGET: 42640 €
PRINCIPAL INVESTIGATOR: M. Sodupe

17. PROJECT TITLE: Activación de biomoléculas por cationes metálicos y superficies siliceas
FUNDING AGENCY: MICINN CTQ2008-06381/BQU
LENGTH FROM: 2009 TO: 2011
BUDGET: 149314 €
PRINCIPAL INVESTIGATOR: M. Sodupe

18. PROJECT TITLE: Silica surface properties and their influence in adsorption processes from computational simulations
FUYNDING AGENCY: Mobility call for visitor professors, MEC. SAB2011-0033
LENGTH FROM: April 2012 TO: august 2012
DUDGET: 9500 €
HOST GROUP INVESTIGATOR: Mariona Sodupe
VISITANT PROFESSOR: Piero Ugliengo

19. PROJECT TITLE: Estudios computacionales de estructura y reactividad química. Aplicación a sistemas de interés biológico.
FUNDING AGENCY: MICINN CTQ2011-24847/BQU
LENGTH FROM: 2012 TO: 2015
BUDGET: 116000 €
PRINCIPAL INVESTIGATOR: Mariona Sodupe

20. PROJECT TITLE: ICREA Academia, 2011
BUDGET: ICREA, Institució Catalana de Recerca i Estudis Avançats
FROM:2011 TO: 2015
BUDGET: 125000
PRINCIPAL INVESTIGATOR: Mariona Sodupe

PUBLICATIONS

ResearcherID: E-9352-2013

152 publications, 6 book chapters

ISI indicators: 3900 citations, h-index = 35, Average citation per item = 26

Articles

[1] M. Sodupe, A. Prenafeta, J. M. Lluch, A. Oliva, J. Bertran, A theoretical study of the reaction of iron ion (Fe^+) (^6D) with hydrogen molecule, *THEOCHEM* **1988**, *43*, 409-414.

[2] E. Wunsch, M. Sodupe, J. M. Lluch, A. Oliva, J. Bertran, Theoretical study of the addition of bromine atoms to monosubstituted and disubstituted derivatives of ethylene, *THEOCHEM* **1988**, *47*, 225-232.

[3] M. Sodupe, J. M. Lluch, A. Oliva, J. Bertran, Theoretical study of the conformational preferences in the Cl_4W:CH2 complex, *Organometallics* **1989**, *8*, 1837-1841.

[4] M. Sodupe, J. M. Lluch, A. Oliva, F. Illas, J. Rubio, Ground and low-lying states of FeH^+ as derived from ab initio self-consistent field and configuration interaction calculations, *J. Chem. Phys.* **1989**, *90*, 6436-6442.

[5] M. Sodupe, A. Oliva, J. Bertran, J. J. Dannenberg, An AM1 and MNDO theoretical study of the Diels-Alder reaction between β-angelica lactone and cyclopentadiene, *J. Org. Chem.* **1989**, *54*, 2488-2490.

[6] M. Sodupe, J. M. Lluch, A. Oliva, F. Illas, J. Rubio, Ab initio study of the ground and low-lying states of iron hydride (FeH), *J. Chem. Phys.* **1990**, *92*, 2478-2480.

[7] M. Sodupe, E. Wunsch, J. M. Lluch, A. Oliva, J. Bertran, MNDO study of the radical addition of hydrogen halides to ethylene and propene, *THEOCHEM* **1990**, *64*, 213-221.

[8] V. Branchadell, M. Sodupe, R. M. Ortuno, A. Oliva, D. Gomez-Pardo, A. Guingant, J. D'Angelo, Diels-Alder cycloadditions of electron-rich, electron-deficient, and push-pull dienes with cyclic dienophiles: high-pressure-induced reactions and theoretical calculations, *J. Org. Chem.* **1991**, *56*, 4135-4141.

[9] Y. Huang, Y. D. Hill, M. Sodupe, C. W. Bauschlicher, Jr., B. S. Freiser, Chemistry of the scandium-benzyne ion in the gas phase, *Inorg. Chem.* **1991**, *30*, 3822-3829.

[10] S. R. Langhoff, C. W. Bauschlicher, Jr., H. Partridge, M. Sodupe, Theoretical study of one and two ammonia molecules bound to the first-row transition metal ions, *J. Phys. Chem.* **1991**, *95*, 10677-10681.

[11] M. Sodupe, C. W. Bauschlicher, Jr., Theoretical study of the bonding of the first- and second-row transition-metal positive ions to acetylene, *J. Phys. Chem.* **1991**, *95*, 8640-8645.

[12] M. Sodupe, C. W. Bauschlicher, Jr., Al(1+)-ligand binding energies, *Chem. Phys. Lett.* **1991**, *181*, 321-326.

[13] M. Sodupe, C. W. Bauschlicher, Jr., H. Partridge, The metal-ligand binding energies for ($Sr(H_2O)^{n+}$), *J. Chem. Phys.* **1991**, *95*, 9422-9423.

[14] M. Sodupe, J. M. Lluch, A. Oliva, J. Bertran, Ab initio study of the reaction between methylene tungsten chloride (Cl4W=CH2) and ethylene, *THEOCHEM* **1991**, *83*, 37-47.

[15] M. Sodupe, J. M. Lluch, A. Oliva, J. Bertran, Ab initio study of the reaction between methylenemolybdenum tetrachloride ($Cl_4Mo=CH_2$) and ethylene, *New J. Chem.* **1991**, *15*, 321-325.

[16] M. Sodupe, J. M. Lluch, A. Oliva, F. Illas, J. Rubio, An ab initio study of the collinear reaction of $Fe^+(^4F)$ and $Fe^+(^6D)$ with molecular hydrogen, *J. Chem. Phys.* **1991**, *94*, 4352-4355.

[17] C. W. Bauschlicher, Jr., H. Partridge, M. Sodupe, S. R. Langhoff, Theoretical study of the alkaline-earth metal superoxides BeO_2 through SrO_2, *J. Phys. Chem.* **1992**, *96*, 9259-9264.

[18] C. W. Bauschlicher, Jr., M. Sodupe, H. Partridge, A theoretical study of the positive and dipositive ions $M(NH_3)_n$ and $M(H_2O)_n$ for M =Mg, Ca or Sr, *J. Chem. Phys.* **1992**, *96*, 4453-4463.

[19] C. W. Bauschlicher, Jr., M. Sodupe, H. Partridge, S. R. Langhoff, Theoretical study of the $^2A_2$-$^2B_2$ separation of the alkali superoxides, *Chem. Phys. Lett.* **1992**,*197*, 213-216.

[20] Y. Huang, Y. D. Hill, M. Sodupe, C. W. Bauschlicher, Jr., B. S. Freiser, Gas-phase chemistry of $Sc(CH_3)^{2+}$ with alkenes: activation of allylic carbon-hydrogen (C-H) bonds by a d^0 system and the migratory insertion of C=C bonds Sc^+-CH_3 bonds, *J. Am. Chem. Soc.* **1992**, *114*, 9106-9111.

[21] H. Partridge, C. W. Bauschlicher, Jr., M. Sodupe, S. R. Langhoff, Theoretical determination of the alkali metal superoxide bond energies, *Chem. Phys. Lett.* **1992**, *195*, 200-206.

[22] H. Partridge, C. W. Bauschlicher, Jr., M. Sodupe, S. R. Langhoff, Comment on: an ab initio study of the ionization of sodium superoxide, *J. Chem. Phys.* **1992**, *96*, 7871.

[23] M. Sodupe, C. W. Bauschlicher, Jr., A theoretical study of the spectroscopy of MgH_2O^+ and $MgCH_3OH^+$, *Chem. Phys. Lett.* **1992**, *195*, 494-499.

[24] M. Sodupe, C. W. Bauschlicher, Jr., S. R. Langhoff, H. Partridge, Theoretical study of the bonding of the first-row transition-metal positive ions to ethylene, *J. Phys. Chem.* **1992**, *96*, 2118-2122. [Erratum to document cited in CA116(13):128993g], *J. Phys. Chem.* **1992**, *96*, 5670.

[25] M. Sodupe, C. W. Bauschlicher, Jr., T. J. Lee, The calculation of the vibrational frequencies of $CuCO^+$, NiCO, and $CuCH_3$, *Chem. Phys. Lett.* **1992**, *189*, 266-272.

[26] M. Sodupe, C. W. Bauschlicher, Jr., H. Partridge, A theoretical study of $Mg(CO_2)_n^+$ and $Sr(CO_2)_n^+$ for n = 1 and 2 and $Mg_2CO_2^+$, *Chem. Phys. Lett.* **1992**, *192*, 185-194.

[27] C. W. Bauschlicher, Jr., S. R. Langhoff, H. Partridge, M. Sodupe, Determination of the structure and bond energies of nickel dioxide and copper dioxide, *J. Phys. Chem.* **1993**, *97*, 856-859.

[28] C. W. Bauschlicher, Jr., M. Sodupe, A study of the ground and low-lying states of $MgCH_4^+$, *Chem. Phys. Lett.* **1993**, *214*, 489-494.

[29] M. Sodupe, C. W. Bauschlicher, Jr., A theoretical study of the spectroscopy of SrH_2O^+ and $SrNH_3^+$, *Chem. Phys. Lett.* **1993**, *212*, 624-630.

[30] M. Sodupe, C. W. Bauschlicher, Jr., The bonding in $FeC_5H_5^+$, *Chem. Phys. Lett.* **1993**, *207*, 19-22.

[31] M. Sodupe, C. W. Bauschlicher, Jr., The bonding in the low-lying states of MgO_2^+, *Chem. Phys. Lett.* **1993**, *203*, 215-219.

[32] M. Sodupe, C. W. Bauschlicher, Jr., A study of the ground and low-lying states of $MgC_2H_2^+$ and $MgC_2H_4^+$, *Chem. Phys.* **1994**, *185*, 163-171.

[33] M. Sodupe, A. Oliva, J. Bertran, Theoretical Study of the Ionization of the H_2O-H_2O, NH_3-H_2O, and FH-H_2O Hydrogen-Bonded Molecules, *J. Am. Chem. Soc.* **1994**, *116*, 8249-8258.

[34] C. W. Bauschlicher, Jr., M. Sodupe, What is the structure of $FeC_5H_6^+$?, *Chem. Phys. Lett.* **1995**, *240*, 526-532.

[35] L. Rodriguez-Santiago, V. Branchadell, M. Sodupe, Theoretical study of the bonding of NO_2 to Cu and Ag, *J. Chem. Phys.***1995**, *103*, 9738-9743.

[36] M. Sodupe, V. Branchadell, A. Oliva, On the Bonding in Sc-CO_2, *J. Phys. Chem.* **1995**, *99*, 8567-8571.

[37] M. Sodupe, A. Oliva, J. Bertran, Theoretical Study of the Ionization of the H_2S-H_2S, PH_3-H_2S, and ClH-H_2S Hydrogen Bonded Molecules, *J. Am. Chem. Soc.* **1995**, *117*, 8416-8421.

[38] L. Rodriguez-Santiago, M. Sodupe, V. Branchadell, Comparison of density functional and coupled cluster methods in the study of metal-ligand systems: Sc-CO_2 and Cu-NO_2, *J. Chem. Phys.* **1996**, *105*, 9966-9971.

[39] M. Sodupe, V. Branchadell, A. Oliva, Theoretical study of the $ScCO_2$ -> OScCO reaction, *THEOCHEM* **1996**, *371*, 79-84.

[40] E. J. Baerends, V. Branchadell, M. Sodupe, Atomic reference energies for density functional calculations, *Chem. Phys. Lett.* **1997**, *265*, 481-489.

[41] M. Sodupe, V. Branchadell, A. Oliva, J. Bertran, Theoretical study of $ScCO_2^+$, *Int. J. Quantum. Chem.* **1997**, *63*, 523-528.

[42] M. Sodupe, V. Branchadell, M. Rosi, C. W. Bauschlicher, Jr., Theoretical Study of M^+-CO_2 and OM^+CO Systems for First Transition Row Metal Atoms, *J. Phys. Chem. A* **1997**, *101*, 7854-7859.

[43] M. Sodupe, A. Oliva, J. Bertran, Theoretical Study of the Ionization of Phenol-Water and Phenol-Ammonia Hydrogen-Bonded Complexes, J. *Phys. Chem.A* **1997**, *101*, 9142-9151.

[44] M. Sodupe, R. Rios, V. Branchadell, T. Nicholas, A. Oliva, J. J. Dannenberg, A Theoretical Study of the Endo/Exo Selectivity of the Diels-Alder Reaction between Cyclopropene and Butadiene, *J. Am. Chem. Soc.* **1997**, *119*, 4232-4238.

[45] J. Bertran, A. Oliva, L. Rodriguez-Santiago, M. Sodupe, Single versus Double Proton-Transfer Reactions in Watson-Crick Base Pair Radical Cations. A Theoretical Study, *J. Am. Chem. Soc.* **1998**, *120*, 8159-8167.

[46] L. Rodriguez-Santiago, M. Sierka, V. Branchadell, M. Sodupe, J. Sauer, Coordination of Cu^+ Ions to Zeolite Frameworks Strongly Enhances Their Ability to Bind NO_2. An ab Initio Density Functional Study, *J. Am. Chem. Soc.* **1998**, *120*, 1545-1551.

[47] L. Rodriguez-Santiago, M. Sodupe, V. Branchadell, Coordination of NO_2 to Alkaline-Earth Metals. A Theoretical Study, *J. Phys. Chem. A* **1998**, *102*, 630-635.

[48] L. Rodriguez-Santiago, X. Solans-Monfort, M. Sodupe, V. Branchadell, Coordination of NO_2 to Cu and Mg in $M(NO_2)_2$ Complexes. A Theoretical Study, *Inorg. Chem.* **1998**, *37*, 4512-4517.

[49] J. Bertran, A. Oliva, L. Rodriguez-Santiago, M. Sodupe, Potential energy profiles of proton transfer processes in cationic clusters, *Atualidades de Fisico-Quimica Organica,*

[based on the Latin American Conference on Physical Organic Chemistry], 4th, Florianopolis, Brazil, Aug., 1998 **1999**, 91-107.

[50] J. Bertran, L. Rodriguez-Santiago, M. Sodupe, The Different Nature of Bonding in Cu^{+}-Glycine and Cu^{2+}-Glycine, *J. Phys. Chem. B* **1999**, *103*, 2310-2317.

[51] M.-P. Habas, F. Mele, M. Sodupe, F. Illas, Density functional cluster model study of bonding and coordination modes of CO2 on Pd(111), *Surf. Sci.* **1999**, *431*, 208-219.

[52] L. Rodriguez-Santiago, M. Sodupe, A. Oliva, J. Bertran, Hydrogen atom or proton transfer in neutral and single positive ions of salicylic acid and related compounds, *J. Am. Chem. Soc.* **1999**, *121*, 8882-8890.

[53] M. Sodupe, J. Bertran, L. Rodriguez-Santiago, E. J. Baerends, Ground State of the $(H_2O)^{2+}$ Radical Cation: DFT versus Post-Hartree-Fock Methods, *J. Phys. Chem. A* **1999**, *103*, 166-170.

[54] S. Pulkkinen, M. Noguera, L. Rodriguez-Santiago, M. Sodupe, J. Bertran, Gas phase intramolecular proton transfer in cationized glycine and chlorine substituted derivatives (M - Gly, M = Na^{+}, Mg^{2+}, Cu^{+}, Ni^{+}, and Cu^{2+}): existence of zwitterionic structures?, *Chemistry--A European Journal* **2000**, *6*, 4393-4399.

[55] L. Rodriguez-Santiago, M. Sodupe, A. Oliva, J. Bertran, Intramolecular Proton Transfer in Glycine Radical Cation, *J. Phys. Chem. A* **2000**, *104*, 1256-1261.

[56] X. Solans-Monfort, V. Branchadell, M. Sodupe, Theoretical Study of the Structure of $ZCu(NO_2)(NO)$. A Proposed Intermediate in the NOx Decomposition by Cu-ZSM-5, *J. Phys. Chem. A* **2000**, *104*, 3225-3230.

[57] J. Bertran, L. Rodriguez-Santiago, M. Sodupe, Inter- and intramolecular proton transfer processes in ionized hydrogen bonded systems, *Trends in Physical Chemistry* **2001**, *8*, 1-19.

[58] M. Noguera, L. Rodriguez-Santiago, M. Sodupe, J. Bertran, Protonation of glycine, serine and cysteine: conformations, proton affinities and intrinsic basicities, *THEOCHEM* **2001**, *537*, 307-318. *(Número dedicado al Prof. S. Fraga)*

[59] L. Rodriguez-Santiago, M. Sodupe, J. Tortajada, Gas-Phase Reactivity of Ni^{+} with Glycine, *J. Phys. Chem. A* **2001**, *105*, 5340-5347.

[60] L. Rodriguez-Santiago, O. Vendrell, I. Tejero, M. Sodupe, J. Bertran, Solvent-assisted catalysis in the enolization of acetaldehyde radical cation, *Chem. Phys. Lett.* **2001**, *334*, 112-118.

[61] S. Simon, J. Bertran, M. Sodupe, Effect of Counterpoise Correction on the Geometries and Vibrational Frequencies of Hydrogen Bonded Systems, *J. Phys. Chem. A* **2001**, *105*, 4359-4364.

[62] J. Bertran, M. Noguera, M. Sodupe, Protonation vs. ionization on intermolecular proton transfer processes in guanine-cytosine Watson-Crick base pair, *Afinidad* **2002**, *59*, 470-478. *(Número especial 500)*

[63] S. Simon, M. Sodupe, J. Bertran, Isomerization versus Fragmentation of Glycine Radical Cation in Gas Phase, *J. Phys. Chem. A* **2002**, *106*, 5697-5702.

[64] X. Solans-Monfort, J. Bertran, V. Branchadell, M. Sodupe, Keto-Enol Isomerization of Acetaldehyde in HZSM5. A Theoretical Study Using the ONIOM2 Method, *J. Phys. Chem. B* **2002**, *106*, 10220-10226.

[65] X. Solans-Monfort, V. Branchadell, M. Sodupe, On the NO Decomposition by Cu-ZSM-5 through the ZCu(NO2)(NO) or ZCu(N2O3) Intermediates, *J. Phys. Chem. B* **2002**, *106*, 1372-1379.

[66] X. Solans-Monfort, M. Sodupe, V. Branchadell, Spin-forbidden N_2O dissociation in Cu-ZSM-5, *Chem. Phys. Lett.* **2002**, *368*, 242-246.

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[68] A. Gil, J. Bertran, M. Sodupe, Gas Phase Dissociation Energies of Saturated $AH_n^{\cdot+}$ Radical Cations and AH_n Neutrals (A = Li-F, Na-Cl): Dehydrogenation, Deprotonation, and Formation of $AH^{\cdot+}_{n-2}$ - H_2 Complexes, *J. Am. Chem. Soc.* **2003**, *125*, 7461-7469.

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[71] L. Blancafort, J. Bertran, M. Sodupe, Triplet (π,π^*) Reactivity of the Guanine-Cytosine DNA Base Pair: Benign Deactivation versus Double Tautomerization via Intermolecular Hydrogen Transfer, *J. Am. Chem. Soc.* **2004**, *126*, 12770-12771.

[72] A. Gil, M. Sodupe, J. Bertran, Unusual hydrogen bonds in $[AH_3\text{-}H_3O]^+$ radical cations (A = C, Si, Ge, Sn and Pb) Single-electron hydrogen bond, proton-hydride hydrogen bond and formation of $[H_2AOH_2]^{+\cdot}$ H_2 complexes, *Chem. Phys. Lett.* **2004**, *395*, 27-32.

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[24] M. Sodupe. Redox propertis of Cu2+-Ab complexes., IX Seminarios de Estudios Avanzados sobre Diseño Molecular y Bioinformática, SEADIM 09, Varadero (Cuba) 2013
(Invited Conference)

Organization of scientific conferences and schools

[1] New Theoretical Concepts for Understanding Organic Reactions. NATO advanced study institute, Sant Feliu de Guixols (Girona), 1998, Member of the organizing committee

[2] ESCR Electronic Structure and Chemical Reactivity, an International Symposium in honor of Prof. J. Bertran, Barcelona, 2001, Member the Organizing committee (Secretary)

[3] Prebiotic Chemistry in 2nd Summer School of the Reference Network of Theoretical and Computational Chemistry, Barcelona, 2008, Director

[4] XXVI Reunió de la Xarxa de Referencia de Química Teòrica i Computacional, Barcelona, 2010, Chair of the conference

[5] WATOC satellite "Theoretical modeling of materials", Barcelona, 2011. Member of the organizing committee

Ph. D. Supervised Thesis

[1] "Estudio teórico de la coordinación del NO_2 a metales en fase gas y en la zeolita Cu-ZSM5", Luís Rodríguez Santiago, Universidad Autònoma de Barcelona, 1998

[2] "Modelling of adsorption and catalytic processes in H+ and Cu+ exchanged ZSM5 and CHA zeolites", Xavier Solans Monfort, Universidad Autónoma de Barcelona, 2003

[3] "Proton transfer in DNA base pairs. Potential mutagenic processes", Marc Noguera Julian, Universidad Autónoma de Barcelona, 2006

[4] "Structure and Reactivity of Hydrogen Bonded radical cations: Application to Amino Acids and Peptides", Adriá Gil Mestres, Universidad Autónoma de Barcelona, 2006.

[5] Activation of amino acids and peptides by Cu+ and Cu2+ and aluminosilicates surfaces", Albert Rimola Gibert, Universidad Autónoma de Barcelona, 2007

[6] Activació dels aminoàcids glicina i lisina i dels seus homopèptids per cations de cobalt. Estudis teòrics i d'espectrometria de masses, Erika Constantino Aguilella, Universidad Autónoma de Barcelona, 2008

[7] Hidròlisi de l'enllaç N-glicosidic a la 2'deoxiguanosina. Estudis computacionals", Raquel Ríos Font, Universidad Autónoma de Barcelona, 2008.

[8] Estudio Teórico de la Estructura Electrónica y Molecular de Complejos de Cu1+/2+ y Fe2+/3+ Relevantes en la Enfermedad de Alzheimer, Jorge Alí Torres, Autónoma de Barcelona, 2011

[9] Theoretical study of the surface properties of crystalline and amorphous silica polymorphs Federico Musso, Autónoma de Barcelona 2011.

Present graduate students

Andrea Mirats, Cu complexes in the Alzheimer's disease
Javier Navarro, Silicate surfaces.

Teaching activities

M. Sodupe regularly teaches Spectroscopy, Quantum Chemistry and Basic Chemistry courses at the University Autónoma de Barcelona. In addition, she has participated in PhD courses in the Spanish Interuniversity Master of Theoretical and Computational Chemistry, has supervised nine PhD Thesis and is currently directly supervising two more.