

DOCTORAL THESES

Title: DFT Study of titanium cubane and molybdenum sulphide compounds

PhD student: José-Manuel Gracia Budría

Supervisor: Josep M. Poblet Rius

University: Universitat Rovira i Virgili

Year: 2004

Related papers:

-Freitag K, Gracia J, Martin A, Mena M, Poblet JM, Sarasa JP, Yelamos C. Rhodium/iridium-titanium azaheterometallocubanes. *Chemistry-A European Journal* 7 (2001) 3645-3651.

-Gracia J, Martin A, Mena M, Morales-Varela MD, Poblet JM, Santamaria C. Intercalation of alkali metal cations into layered organotitanium oxides. *Angewandte Chemie-International Edition* 42 (2003) 927-927.

-Abarca A, Galakhov MV, Gracia J, Martin A, Mena M, Poblet JM, Sarasa JP, Yelamos C. Molecular nitrides containing group 4 and 5 metals: Single and double azatitanocubanes. *Chemistry-A European Journal* 9 (2003) 2337-2346.

-Garcia-Castro M, Gracia J, Martin A, Mena M, Poblet JM, Sarasa JP, Yelamos C. Synthetic and theoretical study of the incorporation of metal halides in $[\{\text{Ti}(\eta^5\text{-C}_5\text{Me}_5)(\mu\text{-NH})\}_3(\mu^3\text{-N})]$. *Chemistry-A European Journal* 11 (2005) 1030-1041.

-Gracia J, Poblet JM, Autschbach J, Kazansky LP. Density-functional calculation of the W-183 and O-17 NMR chemical shifts for large polyoxotungstates. *European Journal of Inorganic Chemistry* 6 (2006) 1139-1148.

-Gracia J, Poblet JM, Fernandez JA, Autschbach J, Kazansky LP. DFT calculations of the W-183 NMR chemical shifts in reduced polyoxotungstates. *European Journal of Inorganic Chemistry* 6 (2006) 1149-1154.

Title: Theoretical Characterization of Metallofullerenes

PhD student: Josep Maria Campanera Alsina

Supervisor: Josep M. Poblet Rius

University: Universitat Rovira i Virgili

Year: 2005

Related papers:

- Campanera JM, Bo C, Olmstead MM, Bach AL, Poblet JM. Bonding within the endohedral fullerenes Sc₃N@C-78 and Sc₃N@C-80 as determined by density functional calculations and reexamination of the crystal structure of $\{\text{Sc}_3\text{N}@C-78\} \cdot \text{Co}(\text{OEP}) \cdot 1.5(\text{C}_6\text{H}_6) \cdot 0.3(\text{CHCl}_3)$. *Journal of Physical Chemistry A* 106 (2002) 12356-12364.

- Hayashi A, Xie YM, Poblet JM, Campanera JM, Lebrilla CB, Balch AL. Mass spectrometric and computational studies of heterofullerenes ([C₅₈Pt]⁽⁻⁾, [C₅₉Pt]⁽⁺⁾) obtained by laser ablation of electrochemically deposited films. *Journal of Physical Chemistry A* 108 (2004) 2192-2198.

- Vougioukalakis GC, Prassides K, Campanera JM, Heggie MI, Orfanopoulos M. Open-cage fullerene derivatives with 15-membered-ring orifices. *Journal of Organic Chemistry* 69 (2004) 4524-4526.
- Campanera JM, Munoz J, Vazquez J, Bo C, Poblet JM. Organometallic derivatives of fullerenes: A DFT study of $(\eta(2)\text{-C-x})\{\text{Pt}(\text{PH}_3)_2\}_n$ ($x=60, 70, 84; n=1-6$). *Inorganic Chemistry* 43 (2004) 6815-6821.
- Campanera JM, Heggie MI, Taylor R. Analysis of polyaddition levels in i-SC₃NC₈₀. *Journal of Physical Chemistry B* 109 (2005) 4024-4031.
- Campanera JM, Bo C, Poblet JM. General rule for the stabilization of fullerene cages encapsulating trimetallic nitride templates. *Angewandte Chemie-International Edition* 44 (2005) 7230-7233.
- Campanera JM, Bo C, Balch AL, Ferre J, Poblet JM. Prediction of heterofullerene stabilities: A combined DFT and chemometric study of C₅₆Pt₂, C₅₇Pt₂ and C₈₁Pt₂. *Chemistry-A European Journal* 11 (2005) 2730-2742.
- Rodriguez-Forteza, Antonio; Campanera, Josep M; Cardona, Claudia M; Echegoyen Luis; Poblet Josep M. Dancing on a fullerene surface: Isomerization of Y₃N@(N-ethylpyrrolidino-C-80) from the 6,6 to the 5,6 regioisomer. *Angewandte Chemie-International Edition* 45 (2006) 8176- 8180.
- Campanera JM, Bo C, Poblet JM. Exohedral reactivity of trimetallic nitride template (TNT) endohedral metallofullerenes. *Journal of Organic Chemistry* 71 (2006) 46-54.

Title: In silico studies of the effect of phenolic compounds from grape seed extracts on the activity of phosphoinositide 3-kinase (PI3K) and the farnesoid X receptor (FXR)

PhD student: Montserrat Vaqué Marquès

Supervisor: Gerard Pujadas Anguiano

University: Universitat Rovira i Virgili

Year: 2007

Related papers:

- Vaque, Montserrat; Arola, Anna; Aliagas, Carles; Pujades, Gerard. BDT: an easy-to-use front-end application for automation of massive docking tasks and complex docking strategies with AutoDock. *Bioinformatics* 22 (2006) 1803-1804.
- Vaque, Montserrat; Ardevol, Anna; Blade, Cinta; Salvado, M Josepa; Blay, Mayte; Fernandez-Larrea, Juan; Arola, Lluís; Pujadas, Gerard. Protein-ligand docking: A review of recent advances and future perspectives. *Current Pharmaceutical Analysis* 4 (2008) 1-19.

Title: Estudio teórico de la reactividad de moléculas nitrogenadas sobre superficies metálicas

PhD student: Francisco Ample Navarro

Supervisor: Anna M. Clotet Romeu, Josep Manel Ricart Pla

University: Universitat Rovira i Virgili

Year: 2005

European Doctorate

Related papers:

- Ample F, Curulla D, Fuster F, Clotet A, Ricart JM. Adsorption of CO and CN- on transition metal surfaces: a comparative study of the bonding mechanism. *Surface Science* 497 (2002) 139-154.

- Ample F, Ricart JM, Clotet A, Curulla D, Niemantsverdriet JW. Competitive CN and N₂ formation on Rh(111): a case of entropic stabilization. *Chemical Physics Letters* 385 (2004) 52-54.

- Ample F, Clotet A, Ricart JM. Structure and bonding mechanism of cyanide adsorbed on Pt(111). *Surface Science* 558 (2004) 111-121.

- Ricart JM, Ample F, Clotet A, Curulla D, Niemantsverdriet JW, Paul JF, Perez-Ramirez J. Structure and catalytic processes of N-containing species on Rh(111) from first principles. *Journal of Catalysis* 232 (2005) 179-185.

Title: Modelling unsaturated hydrocarbons on metals: towards understanding catalytic processes

PhD student: Ana Valcárcel Ortí

Supervisor: Anna M. Clotet Romeu, Josep Manel Ricart Pla

University: Universitat Rovira i Virgili

Year: 2005

European Doctorate

Related papers:

- Valcarcel A, Ricart JM, Clotet A, Markovits A, Minot C, Illas F. Structure and bonding of propyne on Cu(111) from density functional periodic and clusters models. *Journal of Chemical Physics* 116 (2002) 1165-1170.

- Valcarcel A, Ricart JM, Clotet A, Markovits A, Minot C, Illas F. Theoretical study of the structure of propene adsorbed on Pt(111). *Surface Science* 519 (2002) 250-258.

- Valcarcel A, Clotet A, Ricart JM, Delbecq F, Sautet P. Comparative DFT study of the adsorption of 1,3-butadiene, 1-butene and 2-cis/trans-butenes on the Pt(111) and Pd(111) surfaces. *Surface Science* 549 (2004) 121-133.

- Valcarcel A, Ricart JM, Illas F, Clotet A. Theoretical interpretation of the IR spectrum of propyne on Cu(111). *Journal of Physical Chemistry B* 108 (2004) 18297- 18305.

- Valcarcel A, Gil A, Ricart JM, Clotet A. Theoretical study of propene adsorbed on sulphated Pt(111). *Chemical Physics Letters* 399 (2004) 295-299.

- Valcarcel A, Clotet A, Ricart JM, Illas F. Comparative theoretical study of the structure and bonding of propyne on the Pt(111) and Pd(111) surfaces. *Chemical Physics* 309 (2005) 33-39.

- Novell-Leruth G, Valcarcel A, Clotet A, Ricart JM, Perez-Ramirez J. DFT characterization of adsorbed NH_x species on Pt(100) and Pt(111) surfaces. *Journal of Physical Chemistry B* 109 (2005) 18061-18069.

- Valcarcel A, Clotet A, Ricart JM, Delbecq F, Sautet P. Selectivity control for the catalytic 1,3-butadiene hydrogenation on Pt(III) and Pd(III) surfaces: Radical versus closed-shell intermediates. *Journal of Physical Chemistry B* 109 (2005) 14175-14182.

- Valcarcel, A; Ricart, Josep M; Clotet, Anna; Illas, Francesc; Markovits, Alexis; Minot, Christian. Theoretical study of dehydrogenation and isomerisation reactions of propylene on Pt(111). *Journal of Catalysis* 241 (2006) 115-122.

- Valcarcel, A; Clotet, Anna; Illas, Francesc; Ricart, Josep M. Adsorption properties and vibrational spectra of propyne adsorbed on Rh(111). Comparison with other (111) metal surfaces. *Physical Chemistry Chemical Physics* 9 (2007) 311-317.

Title: Aplicación de la teoría del funcional de la densidad a la adsorción de moléculas sobre superficies y electrodos metálicos

PhD student: Alfred Gil Arranz

Supervisor: Anna M. Clotet Romeu, Josep Manel Ricart Pla

University: Universitat Rovira i Virgili

Year: 2007

Related papers:

- Gil A, Clotet A, Ricart JM, Illas F, Alvarez B, Rodes A, Feliu JM. Adsorption of CO at palladium monolayers deposited on Pt(111) electrodes. Combined spectroelectrochemical and theoretical study. *Journal of Physical Chemistry B* 105 (2001) 7263-7271.

- Kresse, G; Gil, A; Sautet, P. Significance of single-electron energies for the description of CO on Pt(111). *Physical Review B* 68 (2003) 07340- 07340.

- Gil A, Clotet A, Ricart JM, Kresse G, Garcia-Hernandez M, Rosch N, Sautet P. Site preference of CO chemisorbed on Pt(111) from density functional calculations. *Surface Science* 530 (2003) 71-86.

- Berna A, Rodes A, Feliu JM, Illas F, Gil A, Clotet A, Ricart JM. Structural and spectroelectrochemical study of carbonate and bicarbonate adsorbed on Pt(111) and Pd/Pt(111) electrodes. *Journal of Physical Chemistry B* 108 (2004) 17928- 17939.

- Valcarcel A, Gil A, Ricart JM, Clotet A. Theoretical study of propene adsorbed on sulphated Pt(111). *Chemical Physics Letters* 399 (2004) 295-299.

Title: Determinación ab initio de parámetros de estructura electrónica en óxidos de metales de transición

PhD student: Esther Bordas Casas

Supervisor: Rosa Caballol Lorenzo, Cornelis de Graaf

University: Universitat Rovira i Virgili

Year: 2005

European Doctorate

Related papers:

- Calzado CJ, de Graaf C, Bordas E, Caballol R, Malrieu JP. Four-spin cyclic exchange in spin ladder cuprates. *Physical Review B* 67 (2003) 13240-13240.
- Cabrero J, de Graaf C, Bordas E, Caballol R, Malrieu JP. Role of the coordination of the azido bridge in the magnetic coupling of copper(II) binuclear complexes. *Chemistry-A European Journal* 9 (2003) 2307-2315.
- Bordas E, Caballol R, de Graaf C. Ab initio study of the magnetic coupling in oxalato-bridged dinuclear Ni(II) complexes. *Journal of Molecular Structure-Theochem* 727 (2005) 173-179.
- Bordas E, de Graaf C, Caballol R, Calzado CJ. Electronic structure of CaCu₂O₃: Spin ladder versus one-dimensional spin chain. *Physical Review B* 71 (2005) 04510- 04510.
- Bordas E, Caballol R, de Graaf C, Malrieu JP. Toward a variational treatment of the magnetic coupling between centers with elevated spin moments. *Chemical Physics* 309 (2005) 259-269.
- Bordas, Esther; de Graaf, Coen; Caballol, Rosa; Calzado, Carmen J. Accurate determination of the electronic structure parameters of the spin ladder compounds SrCu₂O₃, Sr₂Cu₃O₅ and CaCu₂O₃. *Theoretical Chemistry Accounts* 116 (2006) 535-548.
- Bordas, E.; Cabrero, J.; de Graaf, C.; Igual, J.; Reguero, M.; Caballol, R. The Difference-Dedicated Configuration Interaction Method: An Accurate Procedure to Calculate Energy Transitions. *Afinidad* 64 (2007) 154-162.

Title: Aplicación del método DDCI al estudio de sistemas radicalarios y mecanismos de reacción

PhD student: Elena Rodríguez Balada

Supervisor: María del Mar Reguero de la Poza, Rosa Caballol Lorenzo

University: Universitat Rovira i Virgili

Year: 2006

Related papers:

- Rodriguez E, Reguero M, Caballol R. The controversial ground state of tetramethyleneethane. An ab initio CI study. *Journal of Physical Chemistry A* 104 (2000) 6253- 6253.
- Rodriguez E, Reguero M. The DDCI method applied to reactivity: Chemiluminescent decomposition of dioxetane. *Journal of Physical Chemistry A* 106 (2002) 504-509.
- Rodriguez E, Caballol R, Reguero M. Ab initio study of the singlet-triplet relative stability of 2,6-dibromo-2',6'-bistrifluoromethyl-diphenylmethylene. *Chemical Physics* 303 (2004) 157-164.
- Gomez, Isabel; Rodriguez, Elena; Reguero, Mar. New insights into the interconversion mechanism between phenol and its isomers. *Journal of Molecular Structure-Theochem* 767 (2006) 11-18.

Title: Codon usage adaptation in prokaryotic genomes

PhD student: Pedro Puigbó Avalos

Supervisor: Santiago García Vallvé

University: Universitat Rovira i Virgili

Year: 2007

European Doctorate

Related papers:

- Guzman E, Palleja A, Puigbo P, Orellana JM, Montero MA, Garcia-Vallve S, Romeu A. Arrangement of sequences in the gamma-proteobacteria replication origin. *Febs Journal* 272 (2005) 112-112.

- Palleja, A.; Puigbo, P.; Guzman, E.; Orellana, J. M.; Marcet, M.; Montero, M. A.; Garcia-Vallve, S.; Romeu, A. Genome organization of genes coding for carbohydrate active enzymes in *Bacteroides* species. *Febs Journal* 273 (2006) 249-250.

- Puigbo, Pere; Garcia-Vallve, Santiago; McInerney, James O. TOPD/FMTS: a new software to compare phylogenetic trees. *Bioinformatics* 23 (2007) 1556-1558.

- Puigbo, Pere; Bravo, Ignacio G.; Garcia-Vallve, Santiago. E-CAI: a novel server to estimate an expected value of Codon Adaptation Index (eCAI). *BMC Bioinformatics* 9 (2008) 65-65.

- Puigbo, Pere; Pasamontes, Alberto; Garcia-Vallve, Santiago. Gaining and losing the thermophilic adaptation in prokaryotes. *Trends in Genetics* 24 (2008) 10-14.

- Puigbo, Pere; Romeu, Antoni; Garcia-Vallve, Santiago. HEG-DB: a database of predicted highly expressed genes in prokaryotic complete genomes under translational selection. *Nucleic Acids Research* 36 (2008) 524-527.

Title: Colloidal and molecular assemblies for bioengineering applications

PhD student: Paula Pescador Álvarez

Supervisor: Ioanis Katakis

University: Universitat Rovira i Virgili

Year: 2007

European Doctorate

Related papers:

- Lopez F, Pescador P, Guell C, Morales ML, Garcia-Parrilla MC, Troncoso AM. Industrial vinegar clarification by cross-flow microfiltration: effect on colour and polyphenol content. *Journal of Food Engineering* 68 (2005) 133-136.

Title: Development of displacement electrochemical immunosensors: The case of 2,4,6-trichloroanisole

PhD student: María Viviana Duarte

Supervisor: Ioanis Katakis

University: Universitat Rovira i Virgili

Year: 2007

European Doctorate

Title: Electrochemically controlled patterning for biosensor arrays

PhD student: Srujan Kumar Dondapati

Supervisor: Ioanis Katakis

University: Universitat Rovira i Virgili

Year: 2006

European Doctorate

Related papers:

- Goud TV, Srinivasulu M, Reddy VLN, Reddy AV, Rao TP, Kumar DS, Murty US, Venkateswarlu Y. Two new bromotyrosine-derived metabolites from the sponge *Psammaphysilla purpurea*. *Chemical & Pharmaceutical Bulletin* 51 (2003) 990-993.

- Acero Sanchez, Josep Lluís A.; Baldrich, Eva; El-Gawad Radi, Abd; Dondapati, Srujan; Lozano Sanchez, Pablo; Katakis, Ioanis; O'Sullivan, Ciara K. Electronic 'off-on' molecular switch for rapid detection of thrombin. *Electroanalysis* 18 (2006) 1957- 1962.

- Dondapati, Srujan Kumar; Montornes, Josep M.; Lozano Sanchez, Pablo; Acero Sanchez, Josep Lluís; O'Sullivan, Ciara; Katakis, Ioanis. Site-directed immobilization of proteins through electrochemical deprotection on electroactive self-assembled monolayers. *Electroanalysis* 18 (2006) 1879- 1884.

- Mir, Monica; Dondapati, Srujan; Vreeke, Mark; Katakis, Ioanis. Enzymatic self-wiring. *Electrochemistry Communications* 9 (2007) 1715-1718.

Title: Oligonucleotide based biosensors for label-free electrochemical protein and DNA detection

PhD student: Mònica Mir Llorente

Supervisor: Ioanis Katakis

University: Universitat Rovira i Virgili

Year: 2006

European Doctorate

Related papers:

- Mir, Monica; Katakis, Ioanis. Towards a fast-responding, label-free electrochemical DNA biosensor. *Analytical and Bioanalytical Chemistry* 381 (2005) 1033-1035.

- Mir, Monica, Katakis, Ioanis. Aptamers as elements of bioelectronic devices. *Molecular Biosystems* 9 (2007) 620-622.

- Mir, Monica; Dondapati, Srujan; Vreeke, Mark; Katakis, Ioanis. Enzymatic self-wiring. *Electrochemistry Communications* 9 (2007) 1715- 1718.

- Mairal, Teresa; Oezalp, Veli Cengiz; Sanchez, Pablo Lozano; Mir, Monica; Katakis, Ioanis; O'Sullivan, Ciara K. Aptamers: molecular tools for analytical applications. *Analytical and Bioanalytical Chemistry* 390 (2008) 989- 1007.

Title: New Techniques for the fabrication of biosensors based on NAD(P)⁺-dependent dehydrogenases

PhD student: Valeri Pavlov

Supervisor: Ioanis Katakis

University: Universitat Rovira i Virgili

Year: 2005

European Doctorate

Related papers:

- Parellada J, Narvaez A, Lopez MA, Dominguez E, Fernandez JJ, Pavlov V, Katakis I. Amperometric immunosensors and enzyme electrodes for environmental applications. *Analytica Chimica Acta* 362 (1998) 47-57.

- Popescu IC, Dominguez E, Narvaez A, Pavlov V, Katakis I. Electrocatalytic oxidation of NADH at graphite electrodes modified with osmium phenanthroline-dione. *Journal of Electroanalytical Chemistry* 464 (1999) 208-214.

- Iyer R, Pavlov V, Katakis I, Bachas LG. Amperometric sensing at high temperature with a "wired" thermostable glucose-6-phosphate dehydrogenase from *Aquifex aeolicus*. *Analytical Chemistry* 15 (2003) 3898- 3901.

Title: Estudio ab initio de mecanismos de reacción en sistemas moleculares fotosensibles

PhD student: Isabel Gómez Lara

Supervisor: María del Mar Reguero de la Poza

University: Universitat Rovira i Virgili

Year: 2005

Related papers:

- Gomez I, Olivella S, Reguero M, Riera A, Sole A. Thermal and photochemical rearrangement of bicyclo[3.1.0]hex-3-en-2-one to the ketonic tautomer of phenol. Computational evidence for the formation of a diradical rather than a zwitterionic intermediate. *Journal of the American Chemical Society* 124 (2002) 15375- 15384.

- Gomez I, Reguero M, Boggio-Pasqua M, Robb MA. Intramolecular charge transfer in 4-aminobenzonitriles does not necessarily need the twist. *Journal of the American Chemical Society* 127 (2005) 7119- 7129.

- Gomez I, Reguero M, Robb MA. Efficient photochemical merocyanine-to-spiropyran ring closure mechanism through an extended conical intersection seam. A model CASSCF/CASPT2 study. *Journal of Physical Chemistry A* 110 (2006) 3986- 3991.

- Gomez, Isabel; Rodriguez, Elena; Reguero, Mar. New insights into the interconversion mechanism between phenol and its isomers. *Journal of Molecular Structure-Theochem* 767 (2006) 11-18.

- Gomez I, Reguero M. Substituent and solvent influence on the nature of the oxyallyl intermediate in the rearrangement of bicyclo[3.1.0]hex-3-en-2-ones. *Molecular Physics* 104 (2006) 889- 901.

- Gomez, Isabel; Mercier, Yannick; Reguero, Mar. Theoretical investigation of luminescence behavior as a function of alkyl chain size in 4-aminobenzonitrile alicyclic derivatives. *Journal of Physical Chemistry A* 110 (2006) 11455- 11461.

Title: Validation of qualitative analytical methods

PhD student: Esther Trullols Soler

Supervisor: Francesc Xavier Rius Ferrús

University: Universitat Rovira i Virgili

Year: 2006

Related papers:

- Trullols, E.; Ruisánchez, I.; Rius, F.X.; Odena, M.; Feliu, M.T. Qualitative method for Determination of Aflatoxin B1 in nuts. *Journal of AOAC Internacional* 87 (2004) 417-423.

- Trullols E, Ruisanchez I, Rius FX. Validation of qualitative analytical methods. *Trac-Trends in Analytical Chemistry* 23 (2004) 137-145.

- Trullols, E.; Ruisánchez, I.; Rius, F.X.; Huguet, J. Validation of qualitative methods of analysis that use control samples. *Trac-Trends in Analytical Chemistry* 24 (2005) 516-524.

- Aguilera, E.; Lucena, R.; Cárdenas, S.; Valcárcel, M.; Trullols, E.; Ruisánchez, I. Robustness in qualitative analysis: a practical approach. *Trac-Trends in Analytical Chemistry* 25 (2006) 621-627.

- Trullols, E.; Ruisánchez, I.; Aguilera, E.; Lucena, R.; Cárdenas, S.; Valcárcel, M. Statistical intervals to validate an autoanalyzer for monitoring the exhaustion of alkaline degreasing baths. *Analytica Chimica Acta* 569 (2006) 260-266.

Title: Seguimiento cuantitativo de reacciones de resinas epoxi mediante espectroscopía de infrarrojo cercano y métodos de resolución de curvas

PhD student: Mariano Enrique Garrido

Supervisor: Francesc Xavier Rius Ferrús

University: Universitat Rovira i Virgili

Year: 2006

Related papers:

- L.A. Mercado, M. Galià, J.A. Reina, M. Garrido, M.S. Larrechi, F.X. Rius. Reactivity of silicon-based epoxy monomers as studied by near-infrared spectroscopy and multivariate curve resolution methods. *Journal of Polymer Science. Part A. Polymer Chemistry* 44 (2006)1447- 1456.

- M. Garrido, M.S. Larrechi, F.X. Rius. Modeling of complex viscosity changes in the curing of epoxy resins from near-infrared spectroscopy and multivariate regression analysis. *Applied Spectroscopy* 68 (2004) 1424-1430.

- M. Garrido, M.S. Larrechi, F.X. Rius, R. Tauler. Calculation of band boundaries of feasible solutions obtained by Multivariate Curve Resolution Alternating Least Squares of multiple runs of a reaction monitored by NIR spectroscopy. *Chemometrics and Intelligent Laboratory Systems* 78 (2005) 111-120.

- M. Garrido, I. Lázaro, M.S. Larrechi, F.X. Rius. Multivariate resolution of rank-deficient near-infrared spectroscopy data from the reaction of curing epoxy resins using the rank augmentation strategy and multivariate curve resolution alternating least squares approach. *Analytica Chimica Acta* 515 (2005) 65-73.

- M. Garrido, M.S. Larrechi, F.X. Rius, J.C. Ronda. Curing reaction of glycidylthioether resins: kinetic model study by near infrared spectroscopy and multivariate curve resolution. *Journal of Polymer Science. Part A. Polymer Chemistry* 44 (2006) 4846- 4856.

- Garrido M, Larrechi MS, Rius FX. Multivariate curve resolution-alternating least squares and kinetic modeling applied to near-infrared data from curing reactions of epoxy resins: Mechanistic approach and estimation of kinetic rate constants. *Applied Spectroscopy* 60 (2006) 171-184.

- Mariano Garrido, María Soledad Larrechi, F. Xavier Rius, Luis Adolfo Mercado, Marina Galià. Kinetic analysis of reactions of Si-based epoxy resins by near-infrared spectroscopy, C-13 NMR and soft-hard modelling. *Analytica Chimica Acta*. 583 (2007) 392- 401.

- M. Garrido, M.S. Larrechi; F.X. Rius. Near infrared spectroscopy and multivariate curve resolution-alternating least squares incorporating ¹³C-NMR information for monitoring epoxy resins reactions. *Journal of Chemometrics* 21 (2007) 263- 269.

- M. Garrido, M.S. Larrechi, F.X. Rius. Validation of the concentration profiles obtained from the near infrared/multivariate curve resolution monitoring of reaction of epoxy resins using high performance liquid chromatography as a reference method. *Analytica Chimica Acta* 585 (2007) 277-285.

Title: New approaches for the design of chiral catalysts. Application in carbonylation reactions

PhD student: Bianca Karelia Muñoz Moreno

Supervisor: Carmen Claver Cabrero

University: Universitat Rovira i Virgili

Year: 2007

European Doctorate

Related papers:

- Guiu E, Munoz B, Castillon S, Claver C. Iridium-catalyzed enantioselective hydrogenation of imines with xylose diphosphite and diphosphinite ligands. *Advanced Synthesis and Catalysis* 345 (2003) 169-171.

- Muñoz B, Marinetti A, Ruiz A, Castillon S, Claver C. Enhanced regioselectivity in palladium-catalysed asymmetric methoxycarbonylation of styrene using phosphitanes as chiral ligands. *Inorganic Chemistry Communications* 8 (2005) 1113- 1115.

- Guiu, Ester; Caporali, Maria; Muñoz, Bianca; Muller, Christian; Lutz, Martin; Spek, Anthony L.; Claver, Carmen; van Leeuwen, Piet W. N. M. Electronic effect of diphosphines on the regioselectivity of the palladium-catalyzed hydroesterification of styrene. *Organometallics* 25 (2006) 3102-3104.

- Muñoz, Bianca K.; Godard, Cyril; Marinetti, Angela; Ruiz, Aurora; Benet-Buchholz, Jordi; Claver, Carmen. Pd-catalysed methoxycarbonylation of vinylarenes using chiral monodentate phosphitanes and phospholane as ligands. Effect of substrate substituents on enantioselectivity. *Dalton Transactions* 47 (2007) 5524-5530.

- Godard, Cyril; Muñoz, Bianca K.; Ruiz, Aurora; Claver, Carmen. Pd-catalysed asymmetric mono- and bis-alkoxycarbonylation of vinylarenes. *Dalton Transactions* 7 (2008) 853-860.

Title: New chiral ligands in asymmetric catalysis. Application in stabilization of metal nanoparticles

PhD student: Maria Rosa Axet Martí

Supervisor: Carmen Claver Cabrero

University: Universitat Rovira i Virgili

Year: 2006

European Doctorate

Related papers:

- Axet MR, Castillon S, Claver C. Rhodium-diphosphite catalysed hydroformylation of allylbenzene and propenylbenzene derivatives. *Inorganica Chimica Acta* 359 (2006) 2973-2979.

- Axet MR, Benet-Buchholz J, Claver C, Sergio S. New C-2-symmetric diphosphite ligands derived from carbohydrates: Effect of the remote stereocenters on asymmetric catalysis. *Advanced Synthesis & Catalysis* 349 (2007) 1983-1998.

- Favier, Isabelle; Gomez, Montserrat; Muller, Guillermo; Axet, M. Rosa; Castillon, Sergio; Claver, Carmen; Jansat, Susanna; Chaudret, Bruno; Philippot, Karine. Palladium catalytic species containing chiral phosphites: Towards a discrimination between molecular and colloidal catalysts. *Advanced Synthesis & Catalysis* 349 (2007) 2459-2469.

Title: Palladium complexes containing diphosphine and sulfonated phosphine ligands for c-c bond forming reactions. catalytic and mechanistic studies

PhD student: Eduardo José García Suárez

Supervisor: Carmen Claver Cabrero

University: Universitat Rovira i Virgili

Year: 2007

Related papers:

- Claudio Bianchini, Peter Brüggeller, Carmen Claver, Georg Czermak, Alexander Dumfort, Andrea Meli, Werner Oberhauser, Eduardo J. Garcia Suarez. Synthesis and characterization of palladium(II) complexes with new diphosphonium-diphosphine and diphosphine ligands. Production of low molecular weight alternating polyketones via catalytic CO/ethene copolymerisation. *Dalton Transactions* 24 (2006) 2964-2973.

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