

OUTPUT

Hardcopies are attached as an Annex, except for articles marked with an asterisk (*): they were included as "submitted" or "in press" in the year 6 report of CIMAT.

PATENT

TITLE: "Compatibilizers to produce nanocomposites, microcomposites and polymeric blends and process of obtaining" **Quijada, R., Yazdani-Pedram, M., Toro, P., Moncada, E.**

In Chile: This Patent application was presented to the Department of Industrial Property Chile with the number CL 2729/2006 and with date 11/10/2006.

In USA: This application will be presented as soon is possible to the USPTO.

TITLE: "Hybrid clay to obtain nanocomposites with application in the automotive, aviation, construction and packing industry among other, and process of obtaining" **Quijada, R., Yazdani-Pedram, M., Toro, P.**

In Chile: This Patent application was presented to the Department of Industrial Property Chile with the number CL 2730/2006 and with date 11/10/2006.

In USA: This application will be presented as soon is possible to the USPTO.

PUBLICATIONS

Águila, G., **Gracia, F.**, Cortés J., and **Araya P.** "Effect of copper species and the presence of reaction products during the complete oxidation of methane on supported CuO catalysts" (Submitted to Applied Catalysis B: Environmental, 2006).

Aguila, G., Guerrero, S., **Gracia, F.**, and **Araya, P.** "Improvement of the thermal stability of hydrous zirconia by post-synthesis treatment with NaOH and NH₄OH solutions". Applied Catalysis A: General **305**, 219 (2006).

Albores P., Slep L.D., Baraldo, L.M., Baggio R., **Garland, M.T.**, and Rentschler E, "Crystal Structure and Electronic and Magnetic Properties of Hexacyanoosmate(III)" Inorg. Chem., **45**, 6, 2361-2363 (2006).

Alvarez -Thon, L, Carrasco-Altamirano H., Catalán Espinoza. L, Gallardo-Araya, C, Cardona-Villada W., and **Ibañez, A.** "1-Ethyl-3-(4-hydroxy-3-methoxyphenyl)-6-methoxy-2-methylindan-5-ol" Acta Cryst. **E62**, o2000–o2002 (2006).

Alvarez -Thon, L., Bustos, C, Schott E., Sanchez C, and **Ibañez, A.** "Double π - π stacking in 2-[(E)-(3,5-dimethylisoxazol-4-yl)diazanyl]benzoic acid" Acta Cryst. . **E62**, o595–o597, (2006).

Alvarez, A., Clement, E., **Soto, R.**, "Confined suspension jet and long-range hydrodynamic interactions: A destabilization scenario" Physics of Fluids **18**, 083301 (2006)

Arias, J.L., Arias, J.I., **Fernandez, M.S.** "Avian eggshell as a template for biomimetic sintesis of new materials" (In press. In: Handbook of Biomineralization, E. Baeuerlein, P. Behrens, M. Epple (eds), **2**, Wiley-VCH, Weinheim, Germany, 2006.)

Arias, J.L., Mann, K., Nys, Y., García-Ruiz, J.M., **Fernandez, M.S.** "Eggshell growth and matriz macromolecules". (In press, In: Handbook of Biomineralization, E. Baeuerlein (ed.) **1**, Wiley-VCH, Weinheim, Germany, 2006).

* Arranz-Andrés, J., Guevara, J.J., **Velilla, T., Quijada, R.**, Benavente, R., Pérez, E., and Cerrada, M.L. "Syndiotactic Polypropylene and its Copolymers with Alpha-Olefins. Effects of Composition and Length of Comonomer". Polymer, **46**, 12287-12297, (2005).

- Baggio, R., Calvo R., **Garland, M.T**, Peña, O, Pereg M, and Rizzi, A. "Gadolinium and Neodymium Citrates: Evidence for Weak Ferromagnetic Exchange between Gadolinium(III) Cations". *Inorg. Chem.*, **44**, 8979-8987 (2005).
- Barja B., Baggio, R. Calvo, R., **Garland, M.T**, Pereg, M., and Rizzi, A. "Gadolinium(III) and europium (III) L-glutamates: Synthesis and characterization " *Inorg. Chim. Acta* **339** 3921-3926. (2006).
- Belmar, J., Jimenez, C., Ortiz, L., **Garland, M.T.**, Baggio, R. "An oximino tautomer of 1-n-decyl-4-hydroxyimino-3-methyl-1H-pyrazol-5(4H)-one" *Acta Cryst.C*, **C62** (2), o76-o78 (2006).
- Bernal R., **Tassius, Ch.**, Geminard, JC., and **Melo, F.**, "Mechanical characterization of elastic membranes: cell mechanics applications". (To be submitted to *Applied Physics Letters*).
- * Bortolozzo, U., **Clerc, M.G, Falcon, C.**, Residori, S. and **Rojas, R.** "Localized states in bistable pattern forming systems" *Phys. Rev. Lett.* **96**, 214501 (2006).
- * **Calvo-Perez, V.**, Ostrovsky, S., Vega, A., Pelikan, J., **Spodine, E.** "A novel example of a chain structure formed by 1,4- dioxane and cobalt(II) links., W. Haase". *Inorg. Chem.*, **45**, 644-649. (2006)
- Calvo-Perez, V.**, Vega, A., **Spodine, E.** "Effect of the organometallic fragment R=CCHCo₂(CO)₆ on the properties of M₂{OOCR}₄ Clusters (M = Mo, Cu)." *Organometallics.*, **25**, 1953-1960. (2006)
- Carrasco-Altamirano H., Catalán- Espinoza. L., Gallardo-Araya, C., Cardona-Villada W., **Ibañez, A.**, and Alvarez -Thon, L. "4-Allyl-2-methoxy-5-nitrophenyl acetate" *Acta Cryst.* **E62**, o1782-o1784, (2006).
- Cattuto, C., Brito, R., Marini Bettolo Marconi, U., Nori, F., and **Soto, R.** "Fluctuation-Induced Casimir Forces in Granular Fluids" *Phys. Rev. Letters* **96** 178002 (2006)
- * **Clerc, M.G., Escaff, D.** and Kenkre, V.M., "Patterns and localized structures in population dynamics", *Phys. Rev.* **E 72**, 056217 (2005).
- Clerc, M.G., Escaff, D.**, "Solitary waves in van der Waals-like transition in fluidized granular matter", *Physica A* **371**, 33 (2006).
- Clerc, M.G.**, Falcón, C. and **Tirapegui, E.** "Front propagation sustained by additive noise" *Phys. Rev.* **E 74**, 011303 (2006).
- * **Clerc, M.G., Tirapegui, E.**, and Trejos, M. "Patterns formation and localized structures in reaction diffusion systems with non Fickian transport" (Accepted in *Physical Review Letters*. 2006).
- Cordero, P.**, and **Risso, D.** "Tiny reversible rearrangement transitions in granular systems" *Physica A* **371**, 37 (2006)
- Cortés, P., Atria A.M., **Garland, M.T** and Baggio, R. "Two oxo complexes with a tetra nuclear [Fe₄(□₃-O)₂]⁺⁸ and trinuclear [Fe₃(□₃-O)₂]⁺⁷ units". *Acta Cryst.* **C62**, m297-m302.
- Cortés, P., Atria, A.M., **Garland, M.T**, and Baggio, R. "Three oxo complexes with a tetra nuclear [Cu(□₂-Cl)₆(□₄-O)] unit". *Acta Cryst.* **C62**, m311-m314.
- Cortés, J., Valencia, E., and **Araya, P.**, "Monte Carlo simulations studies of the catalytic combustion of methane" (Accepted for publication in *Catalysis Letters*, 2006).
- Covarrubias, C.**, García, R., Arriagada, R., Yáñez, J., **Garland, M.T.** "Cr(III) exchange on zeolites obtained from kaolin and natural mordenite". *Microporous and Mesoporous Materials* **88** (1-3), 20-231. (2006).

- Díaz de vivar, M. E., Baggio, S, **Garland, M.T**, and Baggio R. “-Di- μ^3 sulfato- μ^3 O,O':O"; - μ^3 3O,O':O"-bis_aqua[2,4,6-tris(2-pyridyl)-1,3,5-triazine- μ^3 N1,N2,N6]manganese(II)_tetrahydrate” Acta Cryst. **E62**, m141-m143, (2006).
- Dominguez, A.M., **Quijada, R.**, and **Yazdani-Pedram., M.** “Use of Functionalized Metallocene Copolymers from Ethylene and Polar Olefins as Compatibilizers For LDPE/Starch and LDPE/Dextran Blends” Macromol. Mater. Eng., **291**, 962-971, (2006)
- Escobar, C., **Arias, J.L.** “Biomíneralización: Una inspiración biomimética para el diseño de nuevos materiales de uso médico”. Monogr. Electrón. Patol. Vet. **3**(1):20-32. (2006).
- García-Orozco, I.**, **Quijada, R.**, Vera, K., Valderrama, M. “Tris (pyrazolyl) methane Chromium(III) complexes as highly active catalysts for Ethylene Polymerization”. (In press, Journal of Molecular Catalysis A: Chemical, 2006).
- * Gomez, L., Ramírez, H.L., **Neira-Carrillo, A.**, Villalonga, R. “Polyelectrolyte complex formation mediated immobilization of chitosan-invertase neoglycoconjugate on pectin-coated chitin. Bioprocess and Biosystems” Engineering, **28**(6):387-395. (2006).
- Granifo, J, **Garland, M.T**, and Baggio, R. “The effect in the assembly and node nuclearity of the long and rigid character of bis-pyridyl exo- bidentate spacers when react with zinc acetate: Crystal structures of the high nuclearity coordination polymers [Zn7(l4-O)2(OAc)10(3pdb)]_n (3pdb = 1,4-bis(3-pyridyl)-2, 3-diaza-1,3-butadiene) and [Zn7(l4-O)2(OAc)10(4pdb)]_n (4pdb = 1,4-bis(4-pyridyl)-2,3-diaza-1,3-butadiene”. Polyhedron, **25**, 2277-2283 (2006).
- Granifo, J., **Garland, M.T**, Baggio, R. “Two 1D Zn(II) coordination polymers: catena-Poly[[bis(2,4-pentanedionate-2O)-zinc]- μ -1,4-bis(x-pyridyl) -2,3-diaza-1,3-butadiene] (x = 3, 4)”. Acta Cryst. **C62**, m56-m59 (2006).
- Guerrero, J., Fariás, L., Lemus, L., Quintanilla, A., Mena, A., Cortez, L., Baggio, R.F., **Garland, M.T.** “The new Ru(NBD)Cl₂(substituted-2,2'-biquinoline) complexes. Synthesis and characterization” Polyhedron **25** (1), 9-16. (2006)
- * Guerrero, S., **Araya, P.**, and Wolf, E. “Methane oxidation on Pd supported on high surface area zirconia catalysts” Applied Catalysis A: General **298**, 243 (2006).
- Gutiérrez-Oliva, S., Joubert, L., Adamo, C., Bulat, F.A., Zagal J.H., **Toro-Labbé, A.** “Bridging the gap between the topological and orbital description of hydrogen bonding: The case of the formic acid dimer and its sulfur derivatives” Journal of Physical Chemistry A, **110**_5102-5107(2006)
- * **Hamm, E.** and **Melo, F.** "Laser speckle correlation applied to flow field measurements in granular media". Europhysics Letters, (2006).
- Herrera, B., and **Toro-Labbé: A.** “The role of the reaction force in characterizing the mechanism of double proton transfer in the Adenine-Uracil complex”. (In press Journal of Chemical Physics, 2006).
- López-Majada, J.M., Palza, H., Guevara, J.L., **Quijada, R.**, Martínez, M.C., Benavente. R., Pereña, J.M., Pérez, E., and Cerrada, M.L. “Metallocenic Copolymers of Propene and 1-Hexene: Influence of Comonomer Content and Thermal History on the Structure and Mechanical Properties”. Journal of Polymer Science: Part B, **44**, 1253-1267, (2006).
- Majumder. A., Pilet G., **Garland, M.T**, Rodríguez, and Mitra, S. “Synthesis and structural characterisation of three dicyanamide complexes with Mn(II), Zn(II) and Cd(II): Supramolecular architectures by hydrogen bonding” Polyhedron **25** (1), 2550-2558. (2006).
- Martínez, J., **Quijada, R.**, **Toro-Labbé, A.** “Ethylene polymerization with Zirconocene. The conceptual DFT perspective”. (Paper in preparation).

- * Maurel, A., Pagneux, V., **Barra, F.**, and **Lund, F.** "Wave propagation through a random array of pinned dislocations: Velocity change and attenuation in a generalized Granato and Lücke theory" Phys. Rev. B, **72**, 174111 (2005)
- * Maurel, A., Pagneux, V., Barra, F. and **Lund, F.** "Interaction between an elastic wave and a single pinned dislocation" Phys. Rev. B, **72**, 174110 (2005).

- Maurel, A., Pagneux, V., **Barra, F.**, and **Lund, F.** "Multiple scattering from dislocation walls in 3D polycrystals" (Submitted to Journal of the Acoustical Society of America, 2006).

- Melo, F.** "Nuevos Materiales, El Juego de los Atomos". Revista Explora y Diviértete, Boletín N°28 (May 2006).

- Melo, F.** "¿De qué están hechas las cosas?". Revista Explora y Diviértete, Boletín N°28, (May 2006).

- * **Melo, F., Job, S., Santibañez, F.,** and **Tapia, F.** "Experimental evidence of shock mitigation on a Hertzian tapered Chain". Phys. Rev. E **73**, 041305, (2006).

- * **Melo, F., Vivanco, F.,** Fuentes, C. and Apablaza, V. "On draw bodies shapes: from Bergmark Ross to kinematic models" (To appear in International Journal Mechanics and Mining Sciences, 2006).

- Melo, F., Vivanco, F.,** Fuentes, C., and Apablaza, V. "Kinematic model for quasi-static granular displacements in block caving: Dilatancy effects". (Submitted to the International Journal of Rock Mechanics and Mining Science, August 2006).

- Moncada, E., **Quijada, R.,** and **Retuert, J.** "Comparative Effect of Metallocene and Ziegler-Natta Polypropylene on the Exfoliation of Montmorillonite and Hectorite Clays to Obtain of Nanocomposites". (In Press, Journal of Applied Polymer Science, 2006).

- Moncada, E., **Quijada, R.,** Lieberwirth, I., and **Yazdani-Pedram M.** "Use of PP Grafted with Itaconic Acid as new Compatibilizer for PP/Clay Nanocomposites". Macromol. Chem. Phys., **207**, 1376-1386, (2006).

- Moncada, J.L, and, **Toro-Labbe: A.** "A theoretical study of conducting oligomeric systems: the conceptual DFT perspective". (in press Chemical Physics Letters, 2006)

- Morell, C., Grand, A., Gutiérrez-Oliva, S., **Toro-Labbé, A.** "Using the reactivity-selectivity descriptor $\Delta f(r)$ in organic chemistry". Theoretical Aspects of Chemical Reactivity, **19** 101-117. (2006)

- Moya, S. A., Guerrero J, Rodríguez-Nieto, F.J., Wolcan, E., Felix, M.R, Baggio, R., and **Garland, M.T** "Influence of 4-Substituted Pyridine Ligand L' on both the Conformation and Spectroscopic Properties of the (2,2'- Biquinoline- $\square N^1, \square \square N^1$)tricarbonyl(pyridine- $\square \square N^1$)rhenium (1+) Complex $[\text{Re}(\text{CO})_3\text{-}(\text{bqui})(\text{py})]^+$ and its derivatives $[\text{Re}(\text{CO})_3(\text{L})\text{L}']^+$ (L= 2,2'-Biquinoline and 3,3'-(Ethane-1,2-diyl)-2,2'-biquinoline)." Helvetica Chimica Acta , **88**, 2842-2860 (2005).

- * **Mujica, N.,** and Lathrop, D.P. "Hysteretic gravity-wave bifurcation in a highly turbulent swirling flow". Journal of Fluid Mechanics, **551**, 49-62 (2006).

- * Muñoz, J.C., Atria, A.M, Baggio, R., **Garland, M.T.,** Peña, O., and Orrego, C. "Synthesis and magnetic characterization of Ln(III) complexes with 4,4'-bipyridine and crotonato as bridging ligands". Inorg. Chim. Acta **358**, 4027 -4033 (2005).

- Neira-Carrillo, A., Fernandez, M.S.,** Arias, J.I., **Retuert, J., Arias, J.L.** "Obtainment of polymeric materials from polysiloxane-chitosan composites as template for biomimetic crystallization. In: Biomineralization, from Paleontology to Materials Science" J.L. Arias, M.S. Fernandez (eds), (In Press Editorial Universitaria, Santiago, Chile 2006).

- Pabón, E, **Retuert, J.**, and **Quijada, R.** "Synthesis of Mixed Silica Titania by the Sol-Gel Method using Polyethylenimine: Porosity and Catalytic Properties". (In press, Journal of Porous Material, 2006)
- Palza H., **Velilla, T.**, and **Quijada, R.** "Dynamic model of the Homopolymerization of Propylene with the $\text{Me}_2\text{Si}(\text{2-Me-Ind})_2\text{ZrCl}_2$ Catalysts. The Effect of Reaction Variables". Polymer-Plastics Technology & Engineering, **45**, 85-94, (2006).
- * Palza, H., Velilla, T., **Quijada, R.** "Dynamic Model of the Copolymerization of Propylene and 1-Hexene with the $\text{Me}_2\text{Si}(\text{2-Me-Ind})_2\text{ZrCl}_2$ catalytic system: Effect of 1-Hexene Concentration" Polymer-Plastics Technology & Engineering, **45**, 1-9 (2006).
- Paredes-García, V.**, **Venegas-Yazigi, D.**, Latorre, R.O., **Spodine E.** "Electronic properties of mixed valence iron(II,III) dinuclear complexes with carboxylate bridges.". Polyhedron, **25**, 2026-2032. (2006)
- Piasecki, J., and **Soto, R.** "Approach to a non-equilibrium steady state", Physica A 369, 379 (2006)
- * Requejo, F.G., Ramallo-López, J.M., Rosas-Salas, R., Domínguez, J.M., Rodríguez, J.A, Kim, J.Y., and **Quijada, R.** "Xanes/Exafs Study and Catalytic Properties of the Confined Cr Carbonyl-MCM41 System". Catalyst Today, **107-108**, 750-758, (2005).
- Rincón, E., Jaque, P., **Toro-Labbé, A.** "Reaction force analysis of the effect of Mg(II) on the 1,3 intramolecular hydrogen transfer in Thymine". Journal of Physical Chemistry A, **110**, 9478-9485. (2006)
- Ríos-Escudero, A., Villagrán, M., Caruso, F., Muena, J.P., **Spodine, E.**, **Venegas-Yazigi D.**, Massa, L., Todazo, L.J., Zagal, J.H., Cárdenas-Jirón, G., Paez, M., Costamagna J "Electrocatalytic reduction of carbon dioxide induced by bis-(N-R-2-hydroxy-1-naphthaldiminatoE)-copper(II) (R= n-octyl, n-dodecyl). Magnetic and theoretical studies and the X-Ray structure of bis-(N-n-octyl-2-hydroxy-1-naphthaldiminato)-copper(II)". Inorganica Chimica Acta., **359**, 3947-3953. (2006)
- Rodríguez-Navarro, A., Cabral de Melo, C., Batista, N., Morimoto, N., Alvarez-Lloret, P., Ortega-Huertas, M., Fuenzalida, V.M., Arias, J.I., Wiff, J.P., **Arias, J.L.** "Microstructure and crystallographic-texture of giant barnacle (Austromegabalanus psittacus) shell." (In press, J. Struct. Biol. 2006).
- Soto, R.**, and Malek Mansour, M. "Hydrodynamic boundary condition in vibrofluidized granular systems" Physica A 369, 301 (2006)
- Spodine, E.**, **Venegas-Yazigi, D.**, Ushak, S., Le Fur, E., Pivan, J.Y. "Magnetic behaviour of hybrid organo/inorganic compounds with tetranuclear copper(II) units." Physica B. Condensed Matter. **384**, 120-122. (2006)
- Spodine, E.**, **Venegas-Yazigi, D.**, Ushak, S., **Paredes-García, V.**, Saldias, M., Le Fur, E., Pivan, J.Y. "Magnetic properties of hybrid organo-inorganic copper(II) oxovanadate (V) phosphate and phosphonate bridged systems". (Accepted, Polyhedron. 2006).
- Toro, P.**, **Quijada, R.**, Peralta, R., and **Yazdani-Pedram, M.** "Influence Of Grafted Polypropylene On The Mechanical Properties Of Mineral Filled Polypropylene Composites" Journal of Applied Polymer Science, 000, 000-000, (In press, 2006).
- * **Toro, P.**, **Quijada, R.**, **Yazdani-Pedram, M.**, **Arias, J.L.** "Eggshell, a new bio-filler for polypropylene composites" (Submitted to Materials Letters 2006).
- Toro-Labbé, A.**, Gutiérrez-Oliva, S., Murray, J.S., Politzer, P. "A new Perspective on Chemical Reactions: The reaction force and three key point (not just one) along the intrinsic reaction coordinate". (Submitted to Proceeding of the National Academy of Sciences, US)

- Ushak, S., **Spodine, E.**, Le Fur, E., **Venegas-Yazigi, D.**, Pivan, J.Y., Schnelle, W., Cardoso, R., Kniep, R. "Two new hybrid organic/inorganic copper oxovanadium diphosphate: $[\text{Cu}_2 \text{phen}_2 (\text{O}_3\text{PCH}_2\text{PO}_3) (\text{V}_2\text{O}_5) (\text{H}_2\text{O})] \cdot \text{H}_2\text{O}$, $[\text{Cu phen}_2 (\text{O}_3\text{P}(\text{CH}_2)_3\text{PO}_3) (\text{V}_2\text{O}_5)] \cdot \text{C}_3\text{H}_8$. with encapsulated propane molecules. Synthesis, structure and magnetic properties". *Inorganic Chemistry.*, **45**, 5393-5398 (2006).
- Ushak, S., **Spodine, E.**, **Venegas-Yazigi, D.**, Le Fur, E., Pivan J.Y. "Phosphonate based hybrid organic/inorganic open network compounds $[\text{Cu}(\text{bipy})(\text{VO}_2)_2(\text{O}_3\text{PCH}_2\text{PO}_2\text{OH})\text{H}_2\text{O}$ and $[\text{Cu}(\text{bipy})(\text{VO}_2)(\text{O}_3\text{P}(\text{CH}_2)_2\text{PO}_2\text{OH})]1.5\text{H}_2\text{O}$ ". *Microporous & Mesoporous Materials.*, **94**, 50-55. (2006)
- Venegas-Yazigi D.**, Ruiz, E., Cano, J., Alvarez, S. "Theoretical study of the exchange Coupling in a Ni_{12} single-molecule magnet" *Dalton Trans.*, 2643. (2006)
- Venegas-Yazigi, D.**, Cano, J., Ruiz, E., Alvarez, S. "Theoretical study of the electronic properties and exchange coupling in a Ni_4 cubane like single-molecule magnet". *Physica B. Condensed Matter*, **384**, 123-125. (2006)
- Venegas-Yazigi, D.**, Cortés. S., **Paredes-García, V.**, Peña, O. **Ibañez, A**, Baggio R., **Spodine, E.** "Modulating magnetic properties of a macrocyclic dinuclear copper(II) complex: Influence of counteranions on the crystal structure". *Polyhedron* **25**, 2072-2082, (2006)
- Vidal, V.**, Geminard, J.C., Divaux, T., Legrand, D., and **Melo, F.** "Laboratory acoustic revealing seismic sources on volcanoes". (To be submitted to Nature, October 2006).
- Vidal, V.**, Gémard, J.-C., Divoux, T. and **Melo, F.** "Acoustic signal associated with the bursting of a soap film which initially closes and overpressurized cavity". (Submitted to European Physical Journal, June 2006).
- Wiff, J.P., Fuenzalida, V.M., **Arias, J.L.**, **Fernandez, M.S.** "Hydrothermal-electrochemical CaTiO_3 coatings as precursor of a biomimetic calcium phosphate layer" (In press *Materials Letters*). (2006).
- Yave, W., **Quijada, R.**, Lloyd, D.R., Cerrada, M.L., Benavente, R., and Ulbricht, M. "Propylene/1-Hexene Copolymer as a Taylor-made Polypropylene for Membrana Preparation via the Thermally Induced Phase Separation (TIPS) Process". *Macromolecular Materials and Engineering.* **291**, 155-161, (2006).
- * Yave, W., **Quijada, R.**, Ulbricht, M., and Benavente, R. "Syndiotactic Polypropylenes as Potential Materials for the Preparation of Porous Membrana via Thermally Induced phase Separation (TIPS) process". *Polymer*, **46**, 11582-11590 (2005).