

## **Articles in journals, 2007**

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**H. NOT INCLUDED IN JCR (JOURNAL CITATION REPORTS)**

## Articles in journals, 2007

### A. THEORETICAL PHYSICS AND CHEMISTRY: MODELLING AND SIMULATION OF MATERIALS

- 1.- R.G. Amorim, A. Fazzio, A. Antonelli, F.D. Novaes and A.J.R. da Silva  
*Divacancies in graphene and carbon nanotubes*  
**Nano Letters**, 7 (8), (2007), pp. 2459-2462
- 2.- E.R. Hernández and J. Íñiguez  
*First-principles simulations on the nature of the melting line of sodium*  
**Physical Review Letters**, 98 (5), (2007), pp. 055501-1 – 055501-4
- 3.- J.M. Pruneda, V. Ferrari, R. Rurali, P.B. Littlewood, N.A. Spaldin and E. Artacho  
*Ferrodistorive instability at the (001) surface of half-metallic manganites*  
**Physical Review Letters**, 99 (22), (2007), pp. 226101-1 – 226101-4
- 4.- J.M. Pruneda, D. Sánchez-Portal, A. Arnau, J.I. Juaristi and E. Artacho  
*Electronic stopping power in LiF from first principles*  
**Physical Review Letters**, 99 (23), (2007), pp. 235501-1 – 235501-4
- 5.- F. Biaso, M. Geoffroy, E. Canadell, P. Auban-Senzier, E. Levillain, M. Fourmigué and N. Avarvari  
*Intramolecular mixed-valence state through silicon or germanium double bridges in rigid bis(tetrathiafulvalenes)*  
**Chemistry-A European Journal**, 13 (19), (2007), pp. 5394-5400
- 6.- P. Alemany, E. Canadell and A. Fuytes  
*The staging influence on the electronic structure and transport of superconducting sodium-doped hafnium nitride chloride*  
**Journal of Materials Chemistry**, 17 (41), (2007), pp. 4362-4365
- 7.- F. Llovel, L.J. Florusse, C.J. Peters and L.F. Vega  
*Vapor-liquid and critical behavior of binary systems of hydrogen chloride and n-alkanes: Experimental data and Soft-SAFT modeling*  
**Journal of Physical Chemistry B**, 111 (34), (2007), pp. 10180-10188
- 8.- A.R. Akbarzadeh, L. Bellaiche, J. Íñiguez and D. Vanderbilt  
*Theoretical phase diagram of ultrathin films of incipient ferroelectrics*  
**Applied Physics Letters**, 90 (24), (2007), pp. 242918-1 – 242918-3
- 9.- E. Coronado, S. Curreli, C. Giménez-Saiz, C.J. Gómez-García, P. Deplano, M.L. Mercuri, A. Serpe, L. Pilia, C. Faulmann and E. Canadell  
*New BEDT-TTF/[Fe(C<sub>5</sub>O<sub>5</sub>)<sub>3</sub>]<sup>3-</sup> hybrid system: Synthesis, crystal structure, and physical properties of a chirality-induced  $\alpha$  phase and a novel magnetic molecular metal*  
**Inorganic Chemistry**, 46 (11), (2007), pp. 4446-4457

- 10.- C. Herdes, A. Valente, Z. Lin, J. Rocha, J.A.P. Coutinho, F. Medina and L.F. Vega  
*Selective adsorption of volatile organic compounds in micropore aluminum methylphosphonate- $\alpha$ : A combined molecular simulation-experimental approach*  
**Langmuir**, 23 (13), (2007), pp. 7299-7305
- 11.- O. Degtyareva, E.R. Hernández, J. Serrano, M. Somayazulu, H.K. Mao, E. Gregoryanz and R.J. Hemley  
*Vibrational dynamics and stability of the high-pressure chain and ring phases in S and Se*  
**Journal of Chemical Physics**, 126 (8), (2007), pp. 084503-1 – 084503-11
- 12.- A. Olivet and L.F. Vega  
*Optimized molecular force field for sulfur hexafluoride simulations*  
**Journal of Chemical Physics**, 126 (14), (2007), pp. 144502-1 – 144502-11
- 13.- L. Bellaiche, J. Íñiguez, E. Cockayne and B.P. Burton  
*Effects of vacancies on the properties of disordered ferroelectrics: A first-principles study*  
**Physical Review B**, 75 (1), (2007), pp. 014111-1 – 014111-5
- 14.- R.J.C. Batista, P. Ordejón, H. Chacham and E. Artacho  
*Resistive and rectifying effects of pulling gold atoms at thiol-gold nanocontacts*  
**Physical Review B**, 75 (4), (2007), pp. 041402-1 – 041402-4
- 15.- T.A. Abtew and D.A. Drabold  
*Ab initio models of amorphous  $Si_{1-x}Ge_x : H$*   
**Physical Review B**, 75 (4), (2007), pp. 045201-1 – 045201-9
- 16.- E. Machado-Charry, E. Canadell and A. Segura  
*First-principles study of the electronic structure of cubic GaS: Metallic versus insulating polymorphs*  
**Physical Review B**, 75 (4), (2007), pp. 045206-1 – 045206-7
- 17.- E.R. Hernández, S. Janecek, M. Kaczmarek and E. Krotscheck  
*Evolution-operator method for density functional theory*  
**Physical Review B**, 75 (7), (2007), pp. 075108-1 – 075108-12
- 18.- C. Réthoré, A. Madalan, M. Fourmigué, E. Canadell, E.B. Lopes, M. Almeida, R. Clérac and N. Avarvari  
*O $\cdots$ S vs. N $\cdots$ S intramolecular nonbonded interactions in neutral and radical cation salts of TTF-oxazoline derivatives: Synthesis, theoretical investigations, crystalline structures, and physical properties*  
**New Journal of Chemistry**, 31 (8), (2007), pp. 1468-1483
- 19.- J. Íñiguez, W. Zhou and T. Yildirim  
*Vibrational properties of  $TiH_n$  complexes adsorbed on carbon nanostructures*  
**Chemical Physics Letters**, 444 (1-3), (2007), pp. 140-144
- 20.- J.D. Prades, A. Cirera, J.R. Morante, J.M. Pruneda and P. Ordejón  
*Ab initio study of  $NO_x$  compounds adsorption on  $SnO_2$  surface*  
**Sensors and Actuators B-Chemical**, 126 (1), (2007), pp. 62-67

- 21.- A. Olivet, D. Duque and L.F. Vega  
*Analysis of electron interactions in dielectric gases*  
**Journal of Applied Physics**, 101 (2), (2007), pp. 023308-1 – 023308-7
- 22.- Z. Izaola, S. González, L. Elcoro, J.M. Perez-Mato, G. Madariaga and A. García  
*Revision of pyrrhotite structures within a common superspace model*  
**Acta Crystallographica Section B-Structural Science**, 63, (2007), pp. 693-702
- 23.- J. Íñiguez and T. Yildirim  
*Hydrogen-related catalytic effects of Ti and other light transition metals on NaAlH<sub>4</sub> surfaces*  
**Journal of Physics-Condensed Matter**, 19 (1), (2007), pp. 176007-1 – 176007-8
- 24.- F. Llovel and L.F. Vega  
*Phase equilibria, critical behavior and derivative properties of selected n-alkane/n-alkane and n-alkane/1-alkanol mixtures by the crossover soft-SAFT equation of state*  
**Journal of Supercritical Fluids**, 41 (2), (2007), pp. 204-216
- 25.- E. Krotscheck, E.R. Hernández, S. Janecek, M. Kaczmarek and R. Wahl  
*A new real-space algorithm for realistic density functional calculations*  
**European Physical Journal D**, 43 (1-3), (2007), pp. 173-176
- 26.- D. Vignolles, A. Audouard, R.B. Lyubovskii, S.I. Pesotskii, J. Béard, E. Canadell, G.V. Shilov, O.A. Bogdanova, E.I. Zhilayeva and R.N. Lyubovskaya  
*Crystal structure, Fermi surface calculations and Shubnikov-de Haas oscillation spectrum of the organic metal  $\theta$ -(BETS)<sub>4</sub>HgBr<sub>4</sub>(C<sub>6</sub>H<sub>5</sub>Cl) at low temperature*  
**Solid State Sciences**, 9 (12), (2007), pp. 1140-1148
- 27.- J.R. Trindade, A.M.A. Dias, M. Blesic, N. Pedrosa, L.P.N. Rebelo, L.F. Vega, J.A.P. Coutinho and I.M. Marrucho  
*Liquid-liquid equilibrium of (1H,1H,7H-perfluoroheptan-1-ol + perfluoroalkane) binary mixtures*  
**Fluid Phase Equilibria**, 251 (1), (2007), pp. 33-40
- 28.- C. Rey-Castro, A.L. Tormo and L.F. Vega  
*Effect of the flexibility and the anion in the structural and transport properties of ethyl-methyl-imidazolium ionic liquids*  
**Fluid Phase Equilibria**, 256 (1-2), (2007), pp. 62-69
- 29.- D. Vignolles, A. Audouard, V.N. Laukhin, J. Béard, E. Canadell, N.G. Spitsina and E.B. Yagubskii  
*Frequency combinations in the magnetoresistance oscillations spectrum of a linear chain of coupled orbits with a high scattering rate*  
**European Physical Journal B**, 55 (4), (2007), pp. 383-388
- 30.- N. Pedrosa, L.F. Vega, J.A.P. Coutinho and I.M. Marrucho  
*Modeling the phase equilibria of poly(ethylene glycol) binary mixtures with soft-SAFT EoS*  
**Industrial & Engineering Chemistry Research**, 46 (13), (2007), pp. 4678-4685

- 31.- E. Machado, M. Kaczmarek, B. Braida, P. Ordejón, D. Garg, J. Norman and H. Cheng  
*Interaction of copper organometallic precursors with barrier layers of Ti, Ta and W and their nitrides: A first-principles molecular dynamics study*  
**Journal of Molecular Modeling**, 13 (6-7), (2007), pp. 861-864
- 32.- J. Pellicer-Porres, E. Machado-Charry, A. Segura, S. Gilliland, E. Canadell, P. Ordejón, A. Polian, P. Munsch, A. Chevy and N. Guignot  
*GaS and InSe equations of state from single crystal diffraction*  
**Physica Status Solidi B-Basic Solid State Physics**, 244 (1), (2007), pp. 169-173
- 33.- E.R. Hernández, A. Antonelli, L. Colombo and P. Ordejón  
*The calculation of free-energies in semiconductors: Defects, transitions and phase diagrams*  
**Theory of Defects in Semiconductors, Topics in Applied Physics**, 104, (2007), pp. 115-139
- 34.- A.V. Kazakova, N.D. Kushch, L.I. Buravov, E.B. Yagubskii, S.V. Simonov, L.V. Zorina, S.S. Khasanov, R.P. Shibaeva, E. Canadell, J. Yamada and M. Umemiya  
*First radical cation salts of 2,5-bis(1,3-dithian-2-ylidene)-1,3,4,6-tetrathiapentalene (BDA-TTP) with copper(II) metal complex anions:  $\beta$ -(BDA-TTP)<sub>4</sub>Cu<sub>2</sub>Cl<sub>6</sub> and (BDA-TTP)<sub>2</sub>CuCl<sub>4</sub>*  
**Russian Chemical Bulletin**, 56 (1), (2007), pp. 49-55

## B. MAGNETIC MATERIALS

- 35.- L. Abad, V. Laukhin, S. Valencia, A. Gaup, W. Gudat, L. Balcells and B. Martínez  
*Interfacial strain: The driving force for selective orbital occupancy in manganite thin films*  
**Advanced Functional Materials**, 17 (18), (2007), pp. 3918-3925
- 36.- S. Valencia, A. Gaupp, W. Gudat, L.I. Abad, L.I. Balcells and B. Martínez  
*Surface degradation of magnetic properties in manganite thin films proved with magneto-optical techniques in reflection geometry*  
**Applied Physics Letters**, 90 (25), (2007), pp. 252509-1 – 252509-3
- 37.- S. Estradé, J. Arbiol, F. Peiró, L.I. Abad, V. Laukhin, L.I. Balcells and B. Martínez  
*Cationic diffusion in  $La_{2/3}Ca_{1/3}MnO_3$  thin films grown on  $LaAlO_3$  (001) substrates*  
**Applied Physics Letters**, 91 (25), (2007), pp. 252503-1 – 252503-3
- 38.- F. El Hallak, J. van Slageren, J. Gómez-Segura, D. Ruiz-Molina and M. Dressel  
*High-frequency ESR and frequency domain magnetic resonance spectroscopic studies of single molecule magnets in frozen solution*  
**Physical Review B**, 75 (10), (2007), pp. 104403-1 – 104403-5
- 39.- E. Lhotel, V. Simonet, E. Ressouche, B. Canals, D.B. Amabilino, C. Sporer, D. Luneau, J. Veciana and C. Paulsen  
*Subtle competition between ferromagnetic and antiferromagnetic order in a Mn(II)-free radical ferrimagnetic chain*  
**Physical Review B**, 75 (10), (2007), pp. 104429-1 – 104429-11
- 40.- D. Rubi, J. Fontcuberta, A. Calleja, L.I. Aragonès, X.G. Capdevila and M. Segarra  
*Reversible ferromagnetic switching in  $ZnO:(Co, Mn)$  powders*  
**Physical Review B**, 75 (15), (2007), pp. 155322-1 – 155322-6
- 41.- M. Gajek, M. Bibes, F. Wyczisk, M. Varela, J. Fontcuberta and A. Barthélémy  
*Growth and magnetic properties of multiferroic  $La_xBi_{1-x}MnO_3$  thin films*  
**Physical Review B**, 75 (17), (2007), pp. 174417-1 – 174417-7
- 42.- S. Valencia, A. Gaupp, W. Gudat, L.I. Abad, L.I. Balcells and B. Martínez  
*Impact of microstructure on the Mn valence of  $La_{2/3}Ca_{1/3}MnO_3$  thin films*  
**Physical Review B**, 75 (18), (2007), pp. 184431-1 – 184431-11
- 43.- I.C. Infante, F. Sánchez, J. Fontcuberta, M. Wojcik, E. Jedryka, S. Estradé, F. Peiró, J. Arbiol, V. Laukhin and J.P. Espinós  
*Elastic and orbital effects on thickness-dependent properties of manganite thin films*  
**Physical Review B**, 76 (22), (2007), pp. 224415-1 – 224415-12
- 44.- X. Martí, V. Skumryev, V. Laukhin, F. Sánchez, M.V. García-Cuenca, C. Ferrater, M. Varela and J. Fontcuberta  
*Dielectric anomaly and magnetic response of epitaxial orthorhombic  $YMnO_3$  thin films*  
**Journal of Materials Research**, 22 (8), (2007), pp. 2096-2101

- 45.- I.C. Infante, F. Sánchez, J. Fontcuberta, S. Fusil, K. Bouzehouane, G. Herranz, A. Barthélémy, S. Estradé, J. Arbiol, F. Peiró, R.J.O. Mossaneck, M. Abbate and M. Wojcik  
*Structural and functional characterization of (110)-oriented epitaxial  $La_{2/3}Ca_{1/3}MnO_3$  electrodes and  $SrTiO_3$  tunnel barriers*  
**Journal of Applied Physics**, 101 (9), (2007), pp. 093902-1 – 093902-8
- 46.- C. Martínez-Boubeta  
*Effect of the bias current on the magnetic field switching in micrometer  $AlO_x$ -based tunnel junctions*  
**Journal of Applied Physics**, 102 (4), (2007), pp. 043905-1 – 043905-4
- 47.- J.L. García-Muñoz, C. Frontera, P. Beran, N. Bellido, J.S. Lord, C. Ritter and I. Margiolaki  
*Magnetic and electronic properties of  $Bi_{0.75}Ca_{0.25}MnO_3$*   
**Journal of Physics-Condensed Matter**, 19 (40), (2007), pp. 406212-1 – 406212-9
- 48.- V. Laukhin, X. Martí, V. Skumryev, D. Hrabovsky, F. Sánchez, M.V. García-Cuenca, C. Ferrater, M. Varela, U. Lüders, J.F. Bobo and J. Fontcuberta  
*Electric field effects on magnetotransport properties of multiferroic  $Py/YMnO_3/Pt$  heterostructures*  
**Philosophical Magazine Letters**, 87 (3-4), (2007), pp. 183-191
- 49.- F. Rigato, S. Estradé, J. Arbiol, F. Peiró, U. Lüders, X. Martí, F. Sánchez and J. Fontcuberta  
*Strain-induced stabilization of new magnetic spinel structures in epitaxial oxide heterostructures*  
**Materials Science and Engineering B-Solid State Materials for Advanced Technology**, 144 (1-3), (2007), pp. 43-48
- 50.- N. Dix, V. Skumryev, V. Laukhin, L. Fàbrega, F. Sánchez and J. Fontcuberta  
*Sputtering growth and characterization of  $CoFe_2O_4$ - $BaTiO_3$  nanostructures*  
**Materials Science and Engineering B-Solid State Materials for Advanced Technology**, 144 (1-3), (2007), pp. 127-131
- 51.- D. Rubi D, A. Calleja, J. Arbiol, X.G. Capdevila, M. Segarra, L. Aragonès and J. Fontcuberta  
*Structural and magnetic properties of  $ZnO: TM$  ( $TM : Co, Mn$ ) nanopowders*  
**Journal of Magnetism and Magnetic Materials**, 316 (2), (2007), pp. E211-E214
- 52.- C. Frontera, J.L. García-Muñoz, A.E. Carrillo and A. Caneiro  
*Spin state and magnetic interactions of  $Co^{3+}$  in  $PrBaCo_2O_{5.50}$*   
**Journal of Magnetism and Magnetic Materials**, 316 (2), (2007), pp. E731-E733

### C. SUPERCONDUCTING MATERIALS

- 53.- D.-X. Chen, E. Pardo, A. Sánchez, E. Bartolomé, T. Puig and X. Obradors  
*Magnetic properties of a melt-textured  $YBa_2Cu_3O_x$  ring with a perpendicular crack*  
**Applied Physics Letters**, 90 (7), (2007), pp. 072501-1 – 072501-3
- 54.- J. Gutiérrez, T. Puig and X. Obradors  
*Anisotropy and strength of vortex pinning centers in  $YBa_2Cu_3O_{7-x}$  coated conductors*  
**Applied Physics Letters**, 90 (16), (2007), pp. 162514-1 – 162514-3
- 55.- A. Palau, T. Puig, X. Obradors and Ch. Jooss  
*Simultaneous determination of grain and grain-boundary critical currents in  $YBa_2Cu_3O_7$ -coated conductors by magnetic measurements*  
**Physical Review B**, 75 (5), (2007), pp. 054517-1 – 054517-12
- 56.- E. Bartolomé, A. Palau, J. Gutiérrez, X. Granados, A. Pomar, T. Puig, X. Obradors, V. Cambel, J. Soltys, D. Gregusova, D.-X. Chen and A. Sánchez  
*Artificial magnetic granularity effects on patterned epitaxial  $YBa_2Cu_3O_{7-x}$  thin films*  
**Physical Review B**, 76 (9), (2007), pp. 094508-1 – 94508-9
- 57.- S. Morlens, N. Romá, S. Ricart, A. Pomar, T. Puig and X. Obradors  
*Thickness control of solution deposited YBCO superconducting films by use of organic polymeric additives*  
**Journal of Materials Research**, 22 (8), (2007), pp. 2330-2338
- 58.- A. Palau, T. Puig and X. Obradors  
*Grain and grain boundary vortex dynamics in  $YBa_2Cu_3O_{7-\delta}$  coated conductor by ac susceptibility*  
**Journal of Applied Physics**, 102 (7), (2007), pp. 073911-1 – 073911-8
- 59.- J.-P. Savy, D. de Caro, L. Valade, J.-P. Legros, P. Auban-Senzier, C.R. Pasquier, J. Fraxedas and F. Senocq  
*Superconductivity in  $TTF[Ni(dmit)_2]_2$  films*  
**EPL**, 78 (3), (2007), pp. 37005-1 – 37005-5
- 60.- A. Hassini, A. Pomar, J. Gutiérrez, M. Coll, N. Romà, C. Moreno, A. Ruyter, T. Puig and X. Obradors  
*Atomically flat MOD  $La_{0.7}Sr_{0.3}MnO_3$  buffer layers for high critical current  $YBa_2Cu_3O_7$  TFA films*  
**Superconductor Science & Technology**, 20 (9), (2007), pp. S230-S238
- 61.- E. Bartolomé, F. Gömory, X. Granados, T. Puig and X. Obradors  
*Universal correlation between critical current density and normal-state resistivity in porous  $YBa_2Cu_3O_{7-x}$  thin films*  
**Superconductor Science & Technology**, 20 (10), (2007), pp. 895-899
- 62.- D.-X. Chen, E. Bartolomé, E. Pardo, A. Sánchez, B. Bozzo, X. Granados, T. Puig, X. Obradors and H. Claus  
*AC susceptibility of half-half jointed melt-textured YBCO rings*  
**Physica C-Superconductivity and its Applications**, 460-462, (2007), pp. 770-771



- 63.- C. Navau, E. Bartolomé, N. del Valle, D.-X. Chen, E. Pardo, A. Sánchez, T. Puig and X. Obradors  
*Ac susceptibility of bicrystal-like type-II superconducting films*  
**Physica C-Superconductivity and its Applications**, 460-462, (2007), pp. 787-788
- 64.- A. Hassini, A. Pomar, C. Moreno, A. Ruyter, N. Romà, T. Puig and X. Obradors  
*Conducting  $La_{0.7}Sr_{0.3}MnO_3$ -superconducting  $YBa_2Cu_3O_7$  epitaxial bilayers grown by chemical solution deposition*  
**Physica C-Superconductivity and its Applications**, 460-462, (2007), pp. 1357-1358
- 65.- A. Pomar, A. Llordés, M. Gibert, S. Ricart, T. Puig and X. Obradors  
*Tuning the superconducting properties of  $YBa_2Cu_3O_7$  tapes grown by chemical methods*  
**Physica C-Superconductivity and its Applications**, 460-462, (2007), pp. 1401-1404
- 66.- X. Granados, M. Torner, T. Puig and X. Obradors  
*Magnetization of Ferromagnetic-SC heterostructures for trapped field low power motors*  
**IEEE Transactions on Applied Superconductivity**, 17 (2), (2007), pp. 1629-1632
- 67.- J. López, J. Lloberas, R. Maynou, X. Granados, R. Bosch, X. Obradors and R. Torres  
*AC three-phase axial flux motor with magnetized superconductors*  
**IEEE Transactions on Applied Superconductivity**, 17 (2), (2007), pp. 1633-1636
- 68.- P. Diko, X. Granados, B. Bozzo and P. Kulík  
*Oxygenation thermogravimetry of TSMG YBCO bulk superconductor*  
**IEEE Transactions on Applied Superconductivity**, 17 (2), (2007), pp. 2961-2964
- 69.- R. Cobas, S. Muñoz-Pérez, X. Obradors and J. Albino-Aguilar  
*Analysis of the possible influence of crystallographic shear planes on magnetic and superconducting behavior in  $RuSr_2EuCu_2O_8$*   
**IEEE Transactions on Applied Superconductivity**, 17 (2), (2007), pp. 2973-2975
- 70.- E. Bartolomé, C. Navau, A. Sánchez, D.-X. Chen, T. Puig, X. Obradors and V. Cambel  
*Imaging current percolation and ac losses in artificially granular YBCO thin films*  
**IEEE Transactions on Applied Superconductivity**, 17 (2), (2007), pp. 3223-3226

## D. INORGANIC, ORGANOMETALLIC MATERIALS, COORDINATION COMPOUNDS AND HYBRIDS

- 71.- D. Maspoch, D. Ruiz-Molina and J. Veciana  
*Old materials with new tricks: Multifunctional open-framework materials*  
**Chemical Society Reviews**, 36 (5), (2007), pp. 770-818
- 72.- R. Sarangi, S.D. George, D.J. Rudd, R.K. Szilagy, X. Ribas, C. Rovira, M. Almeida, K.O. Hodgson, B. Hedman and E.I. Solomon  
*Sulfur K-edge X-ray absorption spectroscopy as a probe of ligand-metal bond covalency: Metal vs ligand oxidation in copper and nickel dithiolene complexes*  
**Journal of the American Chemical Society**, 129 (8), (2007), pp. 2316-2326
- 73.- J.G. Planas, F. Teixidor, C. Viñas, M.E. Light and M.B. Hursthouse  
*Self-assembly of halogenated cobaltacarborane compounds: Boron-assisted C-H...X-B hydrogen bonds?*  
**Chemistry-A European Journal**, 13 (9), (2007), pp. 2493-2502
- 74.- D. Gutiérrez-Tauste, X. Domènech, C. Domingo and J.A. Ayllón  
*Hexafluorotitanate salts containing organic cations: Use as a reaction medium and precursor to the synthesis of titanium dioxide*  
**Chemical Communications**, (44), (2007), pp. 4659-4661
- 75.- A. González-Campo, C. Viñas, F. Teixidor, R. Núñez, R. Sillanpää and R. Kivekäs  
*Modular construction of neutral and anionic carboranyl-containing carbosilane-based dendrimers*  
**Macromolecules**, 40 (16), (2007), pp. 5644-5652
- 76.- A. Caballero, V. Lloveras, D. Curiel, A. Tárraga, A. Espinosa, R. García, J. Vidal-Gancedo, C. Rovira, K. Wurst, P. Molina and J. Veciana  
*Electroactive thiazole derivatives capped with ferrocenyl units showing charge-transfer transition and selective ion-sensing properties: A combined experimental and theoretical study*  
**Inorganic Chemistry**, 46 (3), (2007), pp. 825-838
- 77.- D. Maspoch, N. Domingo, D. Ruiz-Molina, K. Wurst, J.M. Hernández, F. Lloret, J. Tejada, C. Rovira and J. Veciana  
*First-row transition-metal complexes based on a carboxylate polychlorotriphenylmethyl radical: Trends in metal-radical exchange interactions*  
**Inorganic Chemistry**, 46 (5), (2007), pp. 1627-1633
- 78.- J. Andrés, M. Feliz, J. Fraxedas, V. Hernández, J.T. López-Navarrete, R. Llusar, G. Sauthier, F.R. Sensato, B. Silvi, C. Bo and J.M. Campanera  
*Combined theoretical and experimental analysis of the bonding in the heterobimetallic cubane-type  $Mo_3NiS_4$  and  $Mo_3CuS_4$  core clusters*  
**Inorganic Chemistry**, 46 (6), (2007), pp. 2159-2166
- 79.- L. Palacios, A.G. De La Torre, S. Bruque, J.L. García-Muñoz, S. García-Granda, D. Sheptyakov and M.A.G. Aranda  
*Crystal structures and in-situ formation study of mayenite electrifieds*  
**Inorganic Chemistry**, 46 (10), (2007), pp. 4167-4176

- 80.- A. Garcia-Raso, F.M. Albertí, J.J. Fiol, A. Tasada, M. Barceló-Oliver, E. Molins, D. Escudero, A. Frontera, D. Quiñonero and P.M. Deyà  
*Anion- $\pi$  interactions in bisadenine derivatives: A combined crystallographic and theoretical study*  
**Inorganic Chemistry**, 46 (25), (2007), pp. 10724-10735
- 81.- J.G. Planas, C. Viñas, F. Teixidor, M.E. Light M.B. Hursthouse  
*Polymorphism and phase transformations in cobaltacarborane molecular crystals*  
**Crystengcomm**, 9 (10), (2007), pp. 888-894
- 82.- C. López, S. Pérez, X. Solans, M. Font-Bardía, A. Roig, E. Molins, P.W.N.M. van Leeuwen and G.P.F. van Strijdonck  
*Heterodimetallic palladium(II) complexes with bidentate (N,S) or terdentate (C,N,S)<sup>-</sup> ferrocenyl ligands. The effect of the ligand donor atoms on the regioselectivity of the allylic alkylation of cinnamyl acetate*  
**Organometallics**, 26 (3), (2007), pp. 571-576
- 83.- I. Boyano, M. Bengoechea, I. de Meatza, O. Miguel, I. Cantero, E. Ochoteco, J. Rodríguez, M. Lira-Cantú and P. Gómez-Romero  
*Improvement in the Ppy/V<sub>2</sub>O<sub>5</sub> hybrid as a cathode material for Li ion batteries using PSA as an organic additive*  
**Journal of Power Sources**, 166 (2), (2007), pp. 471-477
- 84.- S. Piñol, M. Morales and F. Espiell  
*Low temperature anode-supported solid oxide fuel cells based on gadolinium doped ceria electrolytes*  
**Journal of Power Sources**, 169 (1), (2007), pp. 2-8
- 85.- J. Canales-Vázquez, J. Ruiz-Morales, D. Marrero-López, J. Peña-Martínez, P. Núñez and P. Gómez-Romero  
*Fe-substituted (La,Sr)TiO<sub>3</sub> as potential electrodes for symmetrical fuel cells (SFCs)*  
**Journal of Power Sources**, 171 (2), (2007), pp. 552-557
- 86.- I. Boyano, M. Bengoechea, I. de Meatza, O. Miguel, I. Cantero, E. Ochoteco, H. Grande, M. Lira-Cantú and P. Gómez-Romero  
*Influence of acids in the Ppy/V<sub>2</sub>O<sub>5</sub> hybrid synthesis and performance as a cathode material*  
**Journal of Power Sources**, 174 (2), (2007), pp. 1206-1211
- 87.- D. Muñoz-Rojas, J.B. Leriche, C. Delacourt, P. Poizot, M.R. Palacín and J.M. Tarascon  
*Development and implementation of a high temperature electrochemical cell for lithium batteries*  
**Electrochemistry Communications**, 9 (4), (2007), pp. 708-712
- 88.- A.K. Cuentas-Gallegos, R. Martínez-Rosales, M. Baibarac, P. Gómez-Romero and M.E. Rincón  
*Electrochemical supercapacitors based on novel hybrid materials made of carbon nanotubes and polyoxometalates*  
**Electrochemistry Communications**, 9 (8), (2007), pp. 2088-2092

- 89.- F. Teixidor, G. Barberà, R. Kivekäs, R. Sillanpää and C. Viñas  
*Water-stable boron-iodinated dicarbollide dianions [7,8-nido-C<sub>2</sub>H<sub>2</sub>B<sub>9</sub>I<sub>9</sub>]<sup>2-</sup> and [7,8-nido-C<sub>2</sub>H<sub>2</sub>B<sub>9</sub>I<sub>8</sub>H]<sup>2-</sup>*  
**Dalton Transactions**, (17), (2007), pp. 1668-1670
- 90.- F. Lerouge, C. Viñas, F. Teixidor, R. Núñez, A. Abreu, E. Xochitiotzi, R. Santillan and N. Farfán  
*High boron content carboranyl-functionalized aryl ether derivatives displaying photoluminescent properties*  
**Dalton Transactions**, (19), (2007), pp. 1898-1903
- 91.- J. Gómez-Segura, J. Campo, I. Imaz, K. Wurst, J. Veciana, P. Gerbier and D. Ruiz-Molina  
*New insights into the thermal stability of Mn<sub>12</sub> clusters: The case of complex [Mn<sub>12</sub>O<sub>12</sub>(O<sub>2</sub>CC≡CH)<sub>16</sub>(H<sub>2</sub>O)<sub>4</sub>]·3H<sub>2</sub>O and its thermolysis derived [Mn<sub>3</sub>(O<sub>2</sub>CC≡CH)<sub>6</sub>(H<sub>2</sub>O)<sub>4</sub>]·2H<sub>2</sub>O complex*  
**Dalton Transactions**, (23), (2007), pp. 2450-2456
- 92.- C. Viñas, A. Laromaine, F. Teixidor, H. Horáková, A. Langauf, R. Vespalec, I. Mata and E. Molins  
*Synthesis and investigation of the boron cluster anion [7-(2'-pyridyl)7,8-nido-dicarbundaecaborate] and its protonated form*  
**Dalton Transactions**, (31), (2007), pp. 3369-3377
- 93.- D. Marrero-López, D. Pérez-Coll, J.C. Ruiz-Morales, J. Canales-Vázquez, M.C. Martín-Sedeño and P. Núñez  
*Synthesis and transport properties in La<sub>2-x</sub>A<sub>x</sub>Mo<sub>2</sub>O<sub>9-δ</sub> (A = Ca<sup>2+</sup>, Sr<sup>2+</sup>, Ba<sup>2+</sup>, K<sup>+</sup>) series*  
**Electrochimica Acta**, 52 (16), (2007), pp. 5219-5231
- 94.- M.A.Santa-Ana, N. Mirabal, E. Benavente, P. Gómez-Romero and G. González  
*Electrochemical behavior of lithium intercalated in a molybdenum disulfide-crown ether nanocomposite*  
**Electrochimica Acta**, 53 (4), (2007), pp. 1432-1438
- 95.- M. Baibarac, I. Baltog, S. Lefrant and P. Gómez-Romero  
*Spectroscopic evidence for the bulk polymerization of N-vinyl carbazole in the presence of single-walled carbon nanotubes*  
**Polymer**, 48 (18), (2007), pp. 5279-5288
- 96.- M. Barceló-Oliver, A. García-Raso, A. Terrón, E. Molins, M.J. Prieto, V. Moreno, J. Martínez, V. Lladó, I. López, A. Gutiérrez and P.V. Escribá  
*Synthesis and mass spectroscopy kinetics of a novel ternary copper(II) complex with cytotoxic activity against cancer cells*  
**Journal of Inorganic Biochemistry**, 101 (4), (2007), pp. 649-659
- 97.- R. Vespalec, A. Langauf, A. Laromaine, C. Viñas and H. Horakova  
*Electrophoretic investigation of the boron cluster anion [7-(2'-pyridyl)-nido-7,8-dicarbundaecaborate] and its protonated zwitterionic product*  
**Journal of Separation Science**, 30 (16), (2007), pp. 2733-2741

- 98.- M. Lira-Cantú, K. Norrman, J.W. Andreasen, N. Casañ-Pastor and F.C. Krebs  
*Detrimental effect of inert atmospheres on hybrid solar cells based on semiconductor oxides*  
**Journal of the Electrochemical Society**, 154 (6), (2007), pp. B508-B513
- 99.- A. Artillo, G. Della Sala, M. De Santis, A. Llordés, S. Ricart and A. Spinella  
*Preparation of organometallic uracil-analogue Fischer carbene complexes: Comparative study of conventional heating vs microwave irradiation*  
**Journal of Organometallic Chemistry**, 692 (6), (2007), pp. 1277-1284
- 100.- G. Della Sala, A. Artillo, S. Ricart and A. Spinella  
*Synthesis of uracil derivatives by oxidation of Fischer tungsten-carbene uracil complexes*  
**Journal of Organometallic Chemistry**, 692 (8), (2007), pp. 1623-1627
- 101.- S. Pérez, C. López, A. Caubet, X. Solans, M. Font-Bardía, M. Gich and E. Molins  
*Versatility in the mode of coordination  $\{(N), (N,O)^-, (C,N), \text{ or } (C,N,O)^2\}$  of  $[(\eta^5-C_5H_5)Fe\{\eta^5-C_5H_4\}-CH=N-(C_6H_4-2OH)]$  to palladium(II)*  
**Journal of Organometallic Chemistry**, 692 (12), (2007), pp. 2402-2414
- 102.- D. Gutiérrez-Tauste, X. Domènech, N. Casañ-Pastor and J.A. Ayllón  
*Characterization of methylene blue/TiO<sub>2</sub> hybrid thin films prepared by the liquid phase deposition (LPD) method: Application for fabrication of light-activated colorimetric oxygen indicators*  
**Journal of Photochemistry and Photobiology A-Chemistry**, 187 (1), (2007), pp. 45-52
- 103.- M. Barceló-Oliver, A. Terrón, A. García-Raso and E. Molins  
*Models for thyroxine: Aromatic iodine-assisted self-assemblies*  
**Polyhedron**, 26 (7), (2007), pp. 1417-1426
- 104.- M.R. Sundberg, R. Uggla, C. Viñas, F. Teixidor, S. Paavola and R. Kivekäs  
*Nature of intramolecular interactions in hypercoordinate C-substituted 1,2-dicarba-closo-dodecaboranes with short P...P distances*  
**Inorganic Chemistry Communications**, 10 (6), (2007), pp. 713-716
- 105.- J. Oró-Solé, V. Meignen, J. Cabana, M.R. Palacín and A. Fuertes  
*Intermediate phases during alkali metal intercalation in HfNCI*  
**Solid State Sciences**, 9 (3-4), (2007), pp. 310-317
- 106.- N. Roques, S. Perruchas, D. Maspoch, A. Datcu, K. Wurst, J.-P. Sutter, C. Rovira and J. Veciana  
*Europium (III) complexes derived from carboxylic-substituted polychlorotriphenylmethyl radicals*  
**Inorganica Chimica Acta**, 360 (13), (2007), pp. 3861-3869
- 107.- D. Belo, M.J. Figueira, J.P.M. Nunes, I.C. Santos, M. Almeida, N. Crivillers and C. Rovira  
*Synthesis and characterization of the novel extended TTF-type donors with thiophenic units*  
**Inorganica Chimica Acta**, 360 (13), (2007), pp.3909-3914

- 108.- J.C. Ruiz-Morales, J. Canales-Vázquez, B. Ballesteros-Pérez, J. Peña-Martínez, D. Marrero-López, J.T.S. Irvine and P. Núñez  
*LSCM-(YSZ-CGO) composites as improved symmetrical electrodes for solid oxide fuel cells*  
**Journal of the European Ceramic Society**, 27 (13-15), (2007), pp. 4223-4227
- 109.- C.A. García-González, A. Hidalgo, J. Fraile, A.M. López-Periago, C. Andrade and C. Domingo  
*Porosity and water permeability study of supercritically carbonated cement pastes involving mineral additions*  
**Industrial & Engineering Chemistry Research**, 46 (8), (2007), pp. 2488-2496
- 110.- E. Rodríguez, R.V. Simoes, A. Roig, E. Molins, N. Nedelko, A. Ślowska-Waniewska, S. Aime, C. Arús, M.E. Cabañas, C. Sanfeliu, S. Cerdán and M.L. García-Martín  
*An iron-based  $T_1$  contrast agent made of iron-phosphate complexes: In vitro and in vivo studies*  
**Magnetic Resonance Materials in Physics Biology and Medicine**, 20 (1), (2007), pp. 27-37
- 111.- A. Hidalgo, S. Petit, C. Domingo, C. Alonso and C. Andrade  
*Microstructural characterization of leaching effects in cement pastes due to neutralisation of their alkaline nature Part I: Portland cement pastes*  
**Cement and Concrete Research**, 37 (1), (2007), pp. 63-70
- 112.- S. Martínez, E. Trepát, M. Moreno-Mañas, R.M. Sebastián, A. Vallribera, I. Mata and E. Molins  
*Nitrogen-nitrogen bond cleavage catalyzed by ruthenium complexes*  
**Arkivoc**, IV, (2007), pp. 170-181

## E. ORGANIC MATERIALS

- 113.- L. Pérez-García and D.B. Amabilino  
*Spontaneous resolution, whence and whither: From enantiomorphous solids to chiral liquid crystals, monolayers and macro- and supra-molecular polymers and assemblies*  
**Chemical Society Reviews**, 36 (6), (2007), pp. 941-967
- 114.- I. Ratera, C. Sporer, D. Ruiz-Molina, N. Ventosa, J. Baggerman, A.M. Brouwer, C. Rovira and J. Veciana  
*Solvent tuning from normal to inverted Marcus region of intramolecular electron transfer in ferrocene-based organic radicals*  
**Journal of the American Chemical Society**, 129 (19), (2007), pp. 6117-6129
- 115.- D. Maspoch, N. Domingo, N. Roques, K. Wurst, J. Tejada, C. Rovira, D. Ruiz-Molina and J. Veciana  
*Structural and magnetic modulation of a purely organic open framework by selective guest inclusion*  
**Chemistry-A European Journal**, 13 (29), (2007), pp. 8153-8163
- 116.- J.P.M. Nunes, M.J. Figueira, D. Belo, I.C. Santos, B. Ribeiro, E.B. Lopes, R.T. Henriques, J. Vidal-Gancedo, J. Veciana, C. Rovira and M. Almeida  
*Transition metal bisdithiolene complexes based on extended ligands with fused tetrathiafulvalene and thiophene moieties: New single-component molecular metals*  
**Chemistry-A European Journal**, 13 (35), (2007), pp. 9841-9849
- 117.- M. Amat, M.M.M. Santos, A.M. Gómez, D. Jokic, E. Molins and J. Bosch  
*Enantioselective spirocyclizations from tryptophan-derived oxazolopiperidone lactams*  
**Organic Letters**, 9 (15), (2007), pp. 2907-2910
- 118.- T.M. Figueira-Duarte, V. Lloveras, J. Vidal-Gancedo, A. Gégout, B. Delavaux-Nicot, R. Welter, J. Veciana, C. Rovira and J.F. Nierengarten  
*Changes in electronic couplings of mixed-valence systems due to through-space intramolecular interactions*  
**Chemical Communications**, (42), (2007), pp. 4345-4347
- 119.- E. Gomar-Nadal, L. Mugica, J. Vidal-Gancedo, J. Casado, J.T.L. Navarrete, J. Veciana, C. Rovira and D.B. Amabilino  
*Synthesis and doping of a multifunctional tetrathiafulvalene-substituted poly(isocyanide)*  
**Macromolecules**, 40 (21), (2007), pp. 7521-7531
- 120.- J.L. Torres, A. Carreras, A. Jiménez, E. Brillas, X. Torrelles, J. Rius and L. Juliá  
*Reducing power of simple polyphenols by electron-transfer reactions using a new stable radical of the PTM series, tris(2,3,5,6-tetrachloro-4-nitrophenyl)methyl radical*  
**Journal of Organic Chemistry**, 72 (10), (2007), pp. 3750-3756
- 121.- M. Amat, O. Lozano, C. Escolano, E. Molins and J. Bosch  
*Enantioselective synthesis of 3,3-disubstituted piperidine derivatives by enolate dialkylation of phenylglycinol-derived oxazolopiperidone lactams*

**Journal of Organic Chemistry**, 72 (12), (2007), pp. 4431-4439

- 122.- M. Amat, M.M.M. Santos, O. Bassas, N. Llor, C. Escolano, A. Gómez-Esque, E. Molins, S.M. Allin, V. McKee and J. Bosch  
*Straightforward methodology for the enantioselective synthesis of benzo[a]- and indolo[2,3-a]quinolizidines*  
**Journal of Organic Chemistry**, 72 (14), (2007), pp. 5193-5201
- 123.- N. Crivillers, M. Mas-Torrent, S.T. Bromley, K. Wurst, J. Veciana and C. Rovira  
*Influence of intermolecular interactions on the formation of tetra(carbomethoxy)-tetrathiafulvalene assemblies*  
**Chemphyschem**, 8 (10), (2007), pp. 1565-1571
- 124.- G. Subías, T. Abbaz, J.M. Fabre and J. Fraxedas  
*Characterization of the anion-ordering transition in (TMTTF)<sub>2</sub>ReO<sub>4</sub> by x-ray absorption and photoemission spectroscopies*  
**Physical Review B**, 76 (8), (2007), pp. 085103-1 – 085103-7
- 125.- A. Garcia-Raso, F.M. Albertí, J.J. Fiol, A. Tasada, M. Barceló-Oliver, E. Molins, D. Escudero, A. Frontera, D. Quiñonero and P.M. Deya  
*A combined experimental and theoretical study of anion- $\pi$  interactions in bis(pyrimidine) salts*  
**European Journal of Organic Chemistry**, (35), (2007), pp. 5821-5825
- 126.- N. Crivillers, N.S. Oxtoby, M. Mas-Torrent, J. Veciana and C. Rovira  
*Improved synthesis of the high-mobility organic semiconductor dithiophene-tetrathiafulvalene*  
**Synthesis-Stuttgart**, (11), (2007), pp. 1621-1623
- 127.- N. Roques, D. Maspoch, A. Datcu, K. Wurst, D. Ruiz-Molina, C. Rovira and J. Veciana  
*Self-assembly of carboxylic substituted PTM radicals: From weak ferromagnetic interactions to robust porous magnets*  
**Polyhedron**, 26 (9-11), (2007), pp. 1934-1948
- 128.- C. Díez-Gil, A. Caballero, I. Ratera, A. Tárraga, P. Molina and J. Veciana  
*Naked-eye and selective detection of mercury (II) ions in mixed aqueous media using a cellulose-based support*  
**Sensors**, 7 (12), (2007), pp. 3481-3488
- 129.- S. Sala, M. Gimeno, M. Cano, M. Muntó, E. Elizondo, N. Ventosa and J. Veciana  
*DELOS compressed fluid technology for the preparation of micro- and nanoparticulate molecular materials: Main features and scale-up*  
**Afinidad**, 64 (529), (2007), pp. 415-419
- 130.- M. Brito-Arias, D. Cruz-Salazar and E. Molins  
*4-nitrophenyl tetra-O-acetyl- $\beta$ -D-glucopyranoside*  
**Acta Crystallographica Section E-Structure Reports Online**, 63, (2007), pp. O359-O360



## F. METHODOLOGIES, CHARACTERIZATION, OPTICAL AND ELECTROCHEMICAL PROPERTIES OF MATERIALS AND CRYSTAL GROWTH

- 131.- M. Casas-Cabanas, J. Canales-Vázquez, J. Rodríguez-Carvajal and M.R. Palacín  
*Deciphering the structural transformations during nickel oxyhydroxide electrode operation*  
**Journal of the American Chemical Society**, 129 (18), (2007), pp. 5840-5842
- 132.- M. Bosman, V.J. Keast, J.L. García-Muñoz, A.J. D'Alfonso, S.D. Findlay and L.J. Allen  
*Two-dimensional mapping of chemical information at atomic resolution*  
**Physical Review Letters**, 99 (8), (2007), pp. 086102-1 – 086102-4
- 133.- M. Burriel, G. García, M.D. Rossell, A. Figueras, G. Van Tendeloo and J. Santiso  
*Enhanced high-temperature electronic transport properties in nanostructured epitaxial thin films of the  $La_{n+1}Ni_nO_{3n+1}$  Ruddlesden-Popper series ( $n=1, 2, 3, \infty$ )*  
**Chemistry of Materials**, 19 (16), (2007), pp. 4056-4062
- 134.- A. Fragneto, G.M. De Luca, R. Di Capua, U.S. di Uccio, M. Salluzzo, X. Torrelles, T.L. Lee and J. Zegenhagen  
*Ti- and Sr-rich surfaces of  $SrTiO_3$  studied by grazing incidence X-ray diffraction*  
**Applied Physics Letters**, 91 (10), (2007), pp. 101910-1 – 101910-3
- 135.- U. Magdams, X. Torrelles, K. Angermund, H. Gies and J. Rius  
*Crystalline order of a water/glycine film coadsorbed on the (104) calcite surface*  
**Langmuir**, 23 (9), (2007), pp. 4999-5004
- 136.- M. Casas-Cabanas, J. Rodríguez-Carvajal, J. Canales-Vázquez, Y. Lalignant, P. Lacorre and M.R. Palacín  
*Microstructural characterisation of battery materials using powder diffraction data: DIFFaX, FAULTS and SH-FullProf approaches*  
**Journal of Power Sources**, 174 (2), (2007), pp. 414-420
- 137.- D. Heinrich, A.R. Goñi and C. Thomsen  
*Dynamics of magnetic-field-induced clustering in ionic ferrofluids from Raman scattering*  
**Journal of Chemical Physics**, 126 (12), (2007), pp. 124701-1 – 124701-7
- 138.- G. García, R. Doménech-Ferrer, F. Pi, J. Santiso and J. Rodríguez-Viejo  
*Combinatorial synthesis and hydrogenation of Mg/Al libraries prepared by electron beam physical vapor deposition*  
**Journal of Combinatorial Chemistry**, 9 (2), (2007), pp. 230-236
- 139.- A. Pareek, X. Torrelles, J. Rius, U. Magdams and H. Gies  
*Role of water in the surface relaxation of the fluorapatite (100) surface by grazing incidence x-ray diffraction*  
**Physical Review B**, 75 (3), (2007), pp. 035418-1 – 035418-6
- 140.- G. Cabailh, X. Torrelles, R. Lindsay, O. Bikondoa, I. Joumard, J. Zegenhagen and G. Thornton  
*Geometric structure of  $TiO_2(110)(1 \times 1)$ : Achieving experimental consensus*  
**Physical Review B**, 75 (24), (2007), pp. 241403-1 – 241403-4

- 141.- V. Langlais, X. Torrelles, Y. Gauthier and M. De Santis  
*Role of hydrogen interaction in two-dimensional molecular packing with strong molecule-substrate bonding*  
**Physical Review B**, 76 (3), (2007), pp. 035433-1 – 035433-7
- 142.- P.D. Lacharmoise, A. Bernardi, A.R. Goñi, M.I. Alonso and M. Garriga  
*Raman scattering interferences as a probe of vertical coherence in multilayers of carbon-induced Ge quantum dots*  
**Physical Review B**, 76 (15), (2007), pp. 155311-1 – 155311-6
- 143.- I. Mata, E. Molins, I. Alkorta and E. Espinosa  
*Topological properties of the electrostatic potential in weak and moderate N ... H hydrogen bonds*  
**Journal of Physical Chemistry A**, 111 (28), (2007), pp. 6425-6433
- 144.- I. Mata, E. Molins and E. Espinosa  
*Zero-flux surfaces of the electrostatic potential: The border of influence zones of nucleophilic and electrophilic sites in crystalline environment*  
**Journal of Physical Chemistry A**, 111 (39), (2007), pp. 9859-9870
- 145.- J. Llorca, M. Gich and E. Molins  
*The Villalbeta de la Peña meteorite fall: III. Bulk chemistry, porosity, magnetic properties, <sup>57</sup>Fe Mössbauer spectroscopy, and Raman spectroscopy*  
**Meteoritics & Planetary Science**, 42, (2007), pp. A177-A182
- 146.- J. Rius and C. Frontera  
*Application of the constrained S-FFT direct-phasing method to powder diffraction data. XIII*  
**Journal of Applied Crystallography**, 40, (2007), pp. 1035-1038
- 147.- P. Giudici, A.R. Goñi, P.G. Bolcatto, C.R. Proetto, C. Thomsen, K. Eberl and M. Hauser  
*Evidence of breakdown of the spin symmetry in diluted 2D electron gases*  
**EPL**, 77 (3), (2007), pp. 37003-1 – 37003-5
- 148.- E. György, A.P. del Pino, G. Sauthier, A. Figueras, F. Alsina and J. Pascual  
*Structural, morphological and local electric properties of TiO<sub>2</sub> thin films grown by pulsed laser deposition*  
**Journal of Physics D-Applied Physics**, 40 (17), (2007), pp. 5246-5251
- 149.- X. Martí, F. Sánchez, D. Hrabovsky, J. Fontcuberta, V. Laukhin, V. Skumryev, M.V. García-Cuenca, C. Ferrater, M. Varela, U. Lüders, J.F. Bobo, S. Estradé, J. Arbiol and F. Peiró  
*Epitaxial growth of biferroic YMnO<sub>3</sub>(0001) on platinum electrodes*  
**Journal of Crystal Growth**, 299 (2), (2007), pp. 288-294
- 150.- P. Subra-Paternault, C. Roy, D. Vrel, A. Vega-Gonzalez and C. Domingo  
*Solvent effect on tolbutamide crystallization induced by compressed CO<sub>2</sub> as antisolvent*  
**Journal of Crystal Growth**, 309 (1), (2007), pp. 76-85

- 151.- A. Bartasyte, O. Chaix-Pluchery, J. Kreisel, J. Santiso, S. Margueron, M. Boudard, C. Jiménez, A. Abrutis and F.O. Weiss  
*Raman spectroscopy and X-ray diffraction studies of stress effects in PbTiO<sub>3</sub> thin films*  
**IEEE Transactions on Ultrasonics Ferroelectrics and Frequency Control**, 54 (12), (2007), pp. 2623-2631
- 152.- J. Rius, A. Crespi and X. Torrelles  
*A direct phasing method based on the origin-free modulus sum function and the FFT algorithm. XII*  
**Acta Crystallographica Section A**, 63, (2007), pp. 131-134
- 153.- M. Kompitsas, A. Giannoudakos, E. György, G. Sauthier, A. Figueras and I.N. Mihailescu  
*Growth of metal-oxide semiconductor nanocomposite thin films by a dual-laser, dual target deposition system*  
**Thin Solid Films**, 515 (24), (2007), pp. 8582-8585
- 154.- E. György, J. Santiso, A. Figueras, G. Socol and I.N. Mihailescu  
*Biomolecular papain thin films growth by laser techniques*  
**Journal of Materials Science-Materials in Medicine**, 18 (8), (2007), pp. 1643-1647
- 155.- N. McSparran, V. Rico, A. Borrás, A.R. González-Elipe, G. Sauthier, E. György, J. Santiso, G. Garcia, A. Figueras, L. Parafianovic and A. Abrutis  
*Synthesis of undoped and Ni doped InTaO<sub>4</sub> photoactive thin films by metal organic chemical vapor deposition*  
**Surface & Coatings Technology**, 201 (22-23), (2007), pp. 9365-9368
- 156.- E. Gyorgy, S. Grigorescu, G. Socoi, I.N. Mifilailescu, D. Janackovic, A. Dindune, Z. Kanepe, E. Palcevskis, E.L. Zdrentu and S.M. Petrescu  
*Bioactive glass and hydroxyapatite thin films obtained by pulsed laser deposition*  
**Applied Surface Science**, 253 (19), (2007), pp. 7981-7986
- 157.- E. Langenberg, M. Varela, M.V. García-Cuenca, C. Ferrater, F. Sánchez and J. Fontcuberta  
*Thin films in ternary Bi-Mn-O system obtained by pulsed laser deposition*  
**Materials Science and Engineering B-Solid State Materials for Advanced Technology**, 144 (1-3), (2007), pp. 138-142
- 158.- A.N. Hansson, M. Burriel, G. García, S. Linderroth and M.A.J. Somers  
*Oxidation of Fe-22Cr coated with Co<sub>3</sub>O<sub>4</sub>: Microstructure evolution and the effect of growth stresses*  
**Oxidation of Metals**, 68 (1-2), (2007), pp. 23-36
- 159.- J. Fraxedas  
*Growth and characterization of molecular organic crystals and films*  
**Journal of Optoelectronics and Advanced Materials**, 9 (5), (2007), pp. 1322-1328
- 160.- C. Kristukat, A.R. Goñi, K. Potschke, D. Bimberg and C. Thomsen  
*Dependence of the band-gap pressure coefficients of self-assembled InAs/GaAs quantum dots on the quantum dot size*

**Physica Status Solidi B-Basic Solid State Physics**, 244 (1), (2007), pp. 53-58

- 161.- A. Bernardi, J.S. Reparaz, A.R. Goñi, M.I. Alonso and M. Garriga  
*Raman scattering of capped and uncapped carbon-induced Ge dots under hydrostatic pressure*  
**Physica Status Solidi B-Basic Solid State Physics**, 244 (1), (2007), pp. 76-81
- 162.- A. Segura, D. Errandonea, D. Martínez-García, F.J. Manjón, A. Chevy, G. Tobias, P. Ordejón and E. Canadell  
*Transport measurements under pressure in III-IV layered semiconductors*  
**Physica Status Solidi B-Basic Solid State Physics**, 244 (1), (2007), pp. 162-168
- 163.- A. Bernardi, P.D. Lacharmoise, A.R. Goñi, M.I. Alonso, P.O. Vaccaro and N. Saito  
*Strain profile of the wall of semiconductor microtubes: A micro-Raman study*  
**Physica Status Solidi B-Basic Solid State Physics**, 244 (1), (2007), pp. 380-385
- 164.- J.S. Reparaz, A.R. Goñi, M.I. Alonso, M.N. Pérez-Paz and M.C. Tamargo  
*Photoluminescence of CdSe quantum dots with  $Zn_{0.38}Cd_{0.23}Mg_{0.39}Se$  barriers under hydrostatic pressure*  
**Physica Status Solidi B-Basic Solid State Physics**, 244 (1), (2007), pp. 397-401

## G. NANOSTRUCTURED MATERIALS AND NANOSCALE PROPERTIES

- 165.- L.E. Hueso, J.M. Pruneda, V. Ferrari, G. Burnell, J.P. Valdes-Herrera, B.D. Simons, P.B. Littlewood, E. Artacho, A. Fert and N.D. Mathur  
*Transformation of spin information into large electrical signals using carbon nanotubes*  
**Nature**, 445 (7126), (2007), pp. 410-413
- 166.- M. Gajek, M. Bibes, S. Fusil, K. Bouzehouane, J. Fontcuberta, A.E. Barthélémy and A. Fert  
*Tunnel junctions with multiferroic barriers*  
**Nature Materials**, 6 (4), (2007), pp. 296-302
- 167.- J. Gutiérrez, A. Llordés, J. Gázquez, M. Gibert, N. Romà, S. Ricart, A. Pomar, F. Sandiumenge, N. Mestres, T. Puig and X. Obradors  
*Strong isotropic flux pinning in solution-derived  $YBa_2Cu_3O_{7-x}$  nanocomposite superconductor films*  
**Nature Materials**, 6 (5), (2007), pp. 367-373
- 168.- D.B. Amabilino  
*Supramolecular assembly: Nanofibre whirlpools*  
**Nature Materials**, 6 (12), (2007), pp. 924-925
- 169.- J. Puigmarti-Luis, V. Laukhin, A.P. del Pino, J. Vidal-Gancedo, C. Rovira, E. Laukhina and D.B. Amabilino  
*Supramolecular conducting nanowires from organogels*  
**Angewandte Chemie-International Edition**, 46 (1-2), (2007), pp. 238-241
- 170.- N. Crivillers, M. Mas-Torrent, S. Perruchas, N. Roques, J. Vidal-Gancedo, J. Veciana, C. Rovira, L. Basabe-Desmonts, B.J. Ravoo, M. Crego-Calama and D.N. Reinhoudt  
*Self-assembled monolayers of a multifunctional organic radical*  
**Angewandte Chemie-International Edition**, 46 (13), (2007), pp. 2215-2219
- 171.- M. Gibert, T. Puig, X. Obradors, A. Benedetti, F. Sandiumenge and R. Hühne  
*Self-organization of heteroepitaxial  $CeO_2$  nanodots grown from chemical solutions*  
**Advanced Materials**, 19 (22), (2007), pp. 3937-3942
- 172.- A. Cabot, V.F. Puentes, E. Shevchenko, Y. Yin, Ll. Balcells, M.A. Marcus, S.M. Hughes and A.P. Alivisatos  
*Vacancy coalescence during oxidation of iron nanoparticles*  
**Journal of the American Chemical Society**, 129 (34), (2007), pp. 10358-10360
- 173.- E. Martínez-Ferrero, Y. Sakatani, C. Boissière, D. Grosso, A. Fuertes, J. Fraxedas and C. Sanchez  
*Nanostructured titanium oxynitride porous thin films as efficient visible-active photocatalysts*  
**Advanced Functional Materials**, 17 (16), (2007), pp. 3348-3354
- 174.- M. Gich, A. Roig, E. Taboada, E. Molins, C. Bonafos and E. Snoeck  
*Stabilization of metastable phases in spatially restricted fields: The case of the  $Fe_2O_3$  polymorphs*

**Faraday Discussions**, 136, (2007), pp. 345-354

- 175.- J. Gómez-Segura, J. Veciana and D. Ruiz-Molina  
*Advances on the nanostructuration of magnetic molecules on surfaces: the case of single-molecule magnets (SMM)*  
**Chemical Communications**, (36), (2007), pp. 3699-3707
- 176.- D.G. de Oteyza, T.N. Krauss, E. Barrena, S. Sellner, H. Dosch and J.O. Ossó  
*Towards controlled bottom-up architectures in organic heterostructures*  
**Applied Physics Letters**, 90 (24), (2007), pp. 243104-1 – 243104-3
- 177.- J. Verd, A. Uranga, G. Abadal, J. Teva, F. Torres, F. Pérez-Murano, J. Fraxedas, J. Esteve and N. Barniol  
*Monolithic mass sensor fabricated using a conventional technology with attogram resolution in air conditions*  
**Applied Physics Letters**, 91 (1), (2007), pp. 013501-1 – 013501-3
- 178.- J.S. Reparaz, A. Bernardi, A.R. Goñi, P.D. Lacharmoise, M.I. Alonso, M. Garriga, J. Novák and I. Vávra  
*Phonon pressure coefficient as a probe of the strain status of self-assembled quantum dots*  
**Applied Physics Letters**, 91 (8), (2007), pp. 081914-1 – 081914-3
- 179.- C.V. Cojocar, A. Bernardi, J.S. Reparaz, M.I. Alonso, J.M. MacLeod, C. Hamagea and F. Rosei  
*Site-controlled growth of Ge nanostructures on Si(100) via pulsed laser deposition nanostenciling*  
**Applied Physics Letters**, 91 (11), (2007), pp. 113112-1 – 113112-3
- 180.- R. Bachelet, F. Valle, I.C. Infante, F. Sánchez and J. Fontcuberta  
*Step formation, faceting, and bunching in atomically flat SrTiO<sub>3</sub> (110) surfaces*  
**Applied Physics Letters**, 91 (25), (2007), pp. 251904-1 – 251904-3
- 181.- E. Taboada, E. Rodríguez, A. Roig, J. Oró, A. Roch and R.N. Muller  
*Relaxometric and magnetic characterization of ultrasmall iron oxide nanoparticles with high magnetization. Evaluation as potential T<sub>1</sub> magnetic resonance imaging contrast agents for molecular imaging*  
**Langmuir**, 23 (8), (2007), pp. 4583-4588
- 182.- J. Cabana, T. Valdés-Solís, M.R. Palacín, J. Oró-Solé, A. Fuertes, G. Marbán and A.B. Fuertes  
*Enhanced high rate performance of LiMn<sub>2</sub>O<sub>4</sub> spinel nanoparticles synthesized by a hard-template route*  
**Journal of Power Sources**, 166 (2), (2007), pp. 492-498
- 183.- P. Cabrera-Sanfelix, D. Sánchez-Portal, A. Mugarza, T.K. Shimizu, M. Salmeron and A. Arnau  
*Water adsorption on O(2x2)/Ru(0001): STM experiments and first-principles calculations*  
**Physical Review B**, 76 (20), (2007), pp. 205438-1 – 205438-7

- 184.- C. Munuera, E. Barrena and C. Ocal  
*Deciphering structural domains of alkanethiol self-assembled configurations by friction force microscopy*  
**Journal of Physical Chemistry A**, 111 (49), (2007), pp. 12721-12726
- 185.- A. Bernardi, M.I. Alonso, J.S. Reparaz, A.R. Goñi, P.D. Lacharmoise, J.O. Ossó and M. Garriga  
*Evolution of strain and composition during growth and capping of Ge quantum dots with different morphologies*  
**Nanotechnology**, 18 (47), (2007), pp. 475401-1 – 475401-7
- 186.- A. Errachid, D. Caballero, E. Crespo, F. Bessueille, M. Pla-Roca, C.A. Mills, F. Teixidor and J. Samitier  
*Electropolymerization of nano-dimensioned polypyrrole micro-ring arrays on gold substrates prepared using submerged micro-contact printing*  
**Nanotechnology**, 18 (48), (2007), pp. 485301-1 – 485301-8
- 187.- S. Cacchi, C.L. Cotet, G. Fabrizi, G. Forte, A. Goggiamani, L. Martín, S. Martínez, E. Molins, M. Moreno-Mañas, F. Petrucci, A. Roig and A. Vallribera  
*Efficient hydroxycarbonylation of aryl iodides using recoverable and reusable carbon aerogels doped with palladium nanoparticles as catalyst*  
**Tetrahedron**, 63 (11), (2007), pp. 2519-2523
- 188.- J.-P. Savy, D. de Caro, C. Faulmann, L. Valade, M. Almeida, T. Koike, H. Fujiwara, T. Sugimoto, J. Fraxedas, T. Ondarçuhu and C. Pasquier  
*Nanowires of molecule-based charge-transfer salts*  
**New Journal of Chemistry**, 31 (4), (2007), pp. 519-527
- 189.- R. Soler, S. Cacchi, G. Fabrizi, G. Forte, L. Martín, S. Martínez, E. Molins, M. Moreno-Mañas, F. Petrucci, A. Roig, R.M. Sebastian and A. Vallribera  
*Sonogashira cross-coupling using carbon aerogel doped with palladium nanoparticles; A recoverable and reusable catalyst*  
**Synthesis-Stuttgart**, (19), (2007), pp. 3068-3072
- 190.- J. Fraxedas, G. Rius, F. Pérez-Murano and A. Verdager  
*Determining radial breathing mode frequencies of single-walled carbon nanotubes with an atomic force microscope*  
**EPL**, 78 (1), (2007), pp. 16001-1 – 16001-4
- 191.- M. Baibarac, M. Lira-Cantú, J.Oró-Solé, I. Baltog, N. Casañ-Pastor and P. Gómez-Romero  
*Poly(N-vinyl carbazole) and carbon nanotubes based composites and their application to rechargeable lithium batteries*  
**Composites Science and Technology**, 67 (11-12), (2007), pp. 2556-2563
- 192.- M. Gibert, T. Puig and X. Obradors  
*Growth of strain-induced self-assembled BaZrO<sub>3</sub> nanodots from chemical solutions*  
**Surface Science**, 601 (13), (2007), pp. 2680-2683
- 193.- A. Bernardi, M.I. Alonso, A.R. Goñi, J.O. Ossó and M. Garriga  
*Growth dynamics of C-induced Ge dots on Si<sub>1-x</sub>Ge<sub>x</sub> strained layers*  
**Surface Science**, 601 (13), (2007), pp. 2783-2786

- 194.- D.G. de Oteyza, E. Barrena, S. Sellner, J.O. Ossó and H. Dosch  
*Role of the substrate thickness for the structural properties of organic-organic hetero structures*  
**Surface Science**, 601 (18), (2007), pp. 4117-4121



## H. NOT INCLUDED IN JCR (JOURNAL CITATION REPORTS)

- 195.- P.D. Lacharmoise, J.O. Ossó, A.R. Goñi, M.I. Alonso, M. Garriga, E. Barrena, D. G. de Oteyza and H. Dosch  
*SNOM Characterization of self-assembled organic nanocrystals*  
**AIP Conference Proceedings**, 893 (1), (2007), pp. 377-378
- 196.- J. Canales-Vázquez, J.C. Ruiz-Moraley, B. Ballesteros, D. Marrero-López and J.T.S. Irvine  
*Performance of cubic-(La,Sr)TiO<sub>3+δ</sub> as SOFC anodes*  
**Boletín de la Sociedad Española de Cerámica y Vidrio**, 46 (6), (2007), pp. 304-310
- 197.- A. Borrás, C. López, V. Rico, F. Gracia, A.R. González-Elipe, E. Richter, G. Battiston, R. Gerbasi, N. McSparran, G. Sauthier, E. György and A. Figueras  
*Effect of visible and UV illumination on the water contact angle of TiO<sub>2</sub> thin films with incorporated nitrogen*  
**Journal of Physical Chemistry C**, 111 (4), (2007), pp. 1801-1808
- 198.- A.M. Morales-Cas, C. Moya, B. Coto, L.F. Vega and G. Calleja  
*Adsorption of hydrogen and methane mixtures on carbon cylindrical cavities*  
**Journal of Physical Chemistry C**, 111 (17), (2007), pp. 6473-6480
- 199.- J. Casado, M.Z. Zgierski, M.C.R. Delgado, J.T.L. Navarrete, M. Mas-Torrent and C. Rovira  
*Tetrathiafulvalene-based materials for organic field effect transistors. Inspection of their semiconductor properties by means of molecular spectroscopy and quantum chemistry*  
**Journal of Physical Chemistry C**, 111 (27), (2007), pp. 10110-10118
- 200.- D. Duque, B.K. Peterson and L.F. Vega  
*Interaction between coated graphite nanoparticles by molecular simulation*  
**Journal of Physical Chemistry C**, 111 (33), (2007), pp. 12328-12334
- 201.- A. Olivet and L.F. Vega  
*Predictions of transport properties in gaseous mixtures of sulfur hexafluoride and nitrogen*  
**Journal of Physical Chemistry C**, 111 (43), (2007), pp. 16013-16020
- 202.- J.S. Andreu and L.F. Vega  
*Capturing the solubility Behavior of CO<sub>2</sub> in ionic liquids by a simple model*  
**Journal of Physical Chemistry C**, 111 (43), (2007), pp. 16028-16034
- 203.- C. Crespo, S. Gentil, C. Viñas and F. Teixidor  
*Post-overoxidation self-recovery of polypyrrole doped with a metallocarborane anion*  
**Journal of Physical Chemistry C**, 111 (49), (2007), pp. 18381-18386
- 204.- C. Brun, E. Machado-Charry, P. Ordejón, E. Canadell and Z.Z. Wang  
*Inhomogeneities of the CDW vector at the (-201) surface of Quasi-1D blue bronze Rb<sub>0.3</sub>MoO<sub>3</sub>*  
**Journal of Physics: Conference Series**, 61, (2007), pp. 140-146

- 205.- A. Pérez-Tomás, M.R. Jennings, P.A. Mawby, J.A. Covington, P. Godignon, J. Millán and N. Mestres  
*SiC MOSFET channel mobility dependence on substrate doping and temperature considering high density of interface traps*  
**Materials Science Forum**, 556-557, (2007), pp. 835-838
- 206.- M. Placidi, P. Godignon, J. Esteve, N. Mestres, and G. Abadal  
*Fabrication and test of 3C-SiC electrostatic resonators*  
**Materials Science Forum**, 556-557, (2007), pp. 949-952