

A.- THEORETICAL PHYSICS AND CHEMISTRY: MODELLING AND SIMULATION OF MATERIALS**B.- MAGNETIC MATERIALS****C.- SUPERCONDUCTING MATERIALS****D.- INORGANIC AND ORGANOMETALLIC MATERIALS****E.- ORGANIC MATERIALS****F.- METHODOLOGIES, CHARACTERIZATION, OPTICAL PROPERTIES OF MATERIALS AND CRYSTAL GROWTH****A.- THEORETICAL PHYSICS AND CHEMISTRY: MODELLING AND SIMULATION OF MATERIALS**

- 1.- Unexpected Dynamics for Self-Interstitial Clusters in Silicon
Physical Review Letters, 86 (7), (2001), pp. 1247-1250
S.K. Estreicher, M. Gharaibeh, P.A. Fedders and P.Ordejón
- 2.- Ring closure in dioxin formation process: An ab initio molecular dynamics study
Journal of Chemical Physics, 115 (14), (2001), pp. 6401-6405
A.A. Farajian, M. Mikami, P. Ordejón and K. Tanabe
- 3.- Metric-tensor flexible-cell algorithm for isothermal-isobaric molecular dynamics simulations
Journal of Chemical Physics, 115 (22), (2001), pp. 10282-10290
E. Hernández
- 4.- Ab initio study of silicon-multisubstituted neutral and charged fullerenes
Physical Review B, 63, (2001), pp. 085411-1 - 085411-9
C-C Fu, M. Weissmann, M. Machado and P. Ordejón
- 5.- Tubular structures of silicon
Physical Review B, 63, (2001), pp. 193409-1 - 193409-4
G. Seifert, Th. Köhler, H.M. Urbassek, E. Hernández and Th. Frauenheim
- 6.- First-principles study of the origin and nature of ferromagnetism in Ga_{1-x}Mn_xAs
Physical Review B, 63, (2001), pp. 165206-1 - 165206-13
S. Sanvito, P. Ordejón and N.A. Hill
- 7.- Series of (n X 2) Si-rich reconstructions of b-SiC(001): A prospective atomic wire
Physical Review B, 63, (2001), pp. 195306-1 - 195306-9
S.A. Shevlin, A.J. Fisher and E. Hernández
- 8.- Fullerene growth and the role of nonclassical isomers
Physical Review B, 63, (2001), pp. 193403-1 - 193403-4
E. Hernández, P. Ordejón and H. Terrones
- 9.- Phonon eigenvectors of chiral nanotubes
Physical Review B, 64, (2001), pp. 195416-1 - 195416-7
S. Reich, C. Thomsen and P. Ordejón
- 10.- Density-functional calculations of the structures, binding energies, and magnetic moments of Fe clusters with 2 to 17 atoms
Physical Review B, 63, (2001), pp. 205407-1 - 205407-6
O. Diéguez, M.M.G. Alemany, C. Rey, P. Ordejón and L.J. Gallego
- 11.- Self-interstitial-hydrogen complexes in Si

12.- About the evaluation of the local kinetic, potential and total energy densities in closed-shell interactions

Chemical Physics Letters, 336, (2001), pp. 457-461

E. Espinosa, I. Alkorta, I. Rozas, J. Elguero and E. Molins

13.- Surface electronic structure of metastable FeSi(CsCl)(111)

Surface Science, 482-485, (2001), pp. 625-631

J. Junquera, R. Weht and P. Ordejón

14.- Electrons and nuclei of ethylene isomers; a Feynman path integral - ab initio study

Chemical Physics, 264, (2001), pp. 371-400

M.C. Böhm, J. Schulte, E. Hernández and R. Ramírez

15.- Dynamics of interstitial hydrogen molecules in crystalline silicon

Journal of Physics: Condensed Matter, 13, (2001), pp. 6271-6283

S.K. Estreicher, K. Wells, P.A. Fedders and P. Ordejón

16.- Hybrid DNA-gold nanostructured materials: an ab initio approach

Nanotechnology, 12, (2001), pp. 126-131

I.L. Garzón, E. Artacho, M.R. Beltrán, A. García, J. Junquera, K. Michaelian, P. Ordejón, C. Rovira, D. Sánchez-Portal and J.M. Soler

17.- The fascinating dynamics of defects in silicon

Physica B, 308-310 (2001), pp. 308-310

S. K. Estreicher, P.A. Fedders, P. Ordejón

18.- The strange behavior of interstitial H₂ molecules Si and CaAs

Physica B, 308-310, (2001), pp. 202-205

S. K. Estreicher, J. L. McAfee, P. A. Fedders, J. M. Pruneda, P. Ordejón

19.- Vibrational properties of H-related defects in silicon

Physica B, 308-310, (2001), pp. 147-150

J. M. Pruneda, J. Junquera, J. Ferrer, P. Ordejón, S. K. Estreicher

B.- MAGNETIC MATERIALS

20.- Nanoscale Multiphase Separation at La_{2/3}Ca_{1/3}MnO₃/SrTiO₃ Interfaces

Physical Review Letters, 87 (6), (2001), pp. 067210

M. Bibes, Ll. Balcells, S. Valencia, J. Fontcuberta, M. Wojcik, E. Jedryka and S. Nadolski

21.- Cationic ordering control of magnetization in Sr₂FeMoO₆ double perovskite

Applied Physics Letters, 78 (6), (2001), pp. 781-783

Ll. Balcells, J. Navarro, M. Bibes, A. Roig, B. Martínez and J. Fontcuberta

22.- High-temperature orbital and charge ordering in Bi_{1/2}Sr_{1/2}MnO₃

Physical Review B, 63, (2001), pp. 064415

J.L. García-Muñoz, C. Frontera, M.A.G. Aranda, A. Llobet and C. Ritter

23.- Structure and charge-ordering transition in Bi-based bilayered

Bi_{0.44}Ca_{2.56}Mn₂O₇ manganite

Physical Review B, 63, (2001), pp. 144108

Y.L. Qin, J.L. García-Muñoz, H.W. Zandbergen and J.A. Alonso

24.- Pressure effects on the structural phase transition in La_{0.8}MnO₃ single crystals

Physical Review B, 63, (2001), pp. 214417

V. Laukhin, B. Martínez, J. Fontcuberta and Y.M. Mukovskii

25.- Enhancement of antiferromagnetic coupling in the quasi-one-dimensional

Ca₃Co₂O₆ ferrimagnet

Physical Review B, 64, (2001), pp. 012417

B. Martínez, V. Laukhin, M. Hernando, J. Fontcuberta, M. Parras and J.M. González-

26.- Paramagnetic behavior and correlation between high- and low-temperature structural and magnetic transitions in $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ (single - 1/8) single-crystal perovskites

Physical Review B, 64, (2001), pp. 024434

J. Nogués, V. Skumryev, J.S. Muñoz, B. Martínez, J. Fontcuberta, L. Pinsard and A. Revcolevschi

27.- Low-temperature charge and magnetic order of $\text{Bi}_{0.5}\text{Sr}_{0.5}\text{MnO}_3$

Physical Review B, 64, (2001), pp. 054401

C. Frontera, J.L. García-Muñoz, M.A.G. Aranda, C. Ritter, A. Llobet, M. Respaud and J. Vanacken

28.- High-temperature structural evolution of RnO_3 (R = Ho, Y, Er, Lu) perovskites: Charge disproportionation and electronic localization

Physical Review B, 64, (2001), pp. 094102

J.A. Alonso, M.J. Martínez-Lope, M.T. Casais, J.L. García-Muñoz, M.T. Fernández-Díaz and M.A.G. Aranda

29.- Raising the Curie temperature in $\text{Sr}_2\text{FeMoO}_6$ double perovskites by electron doping

Physical Review B, 64, (2001), pp. 092411

J. Navarro, C. Frontera, Ll. Balcells, B. Martínez and J. Fontcuberta

30.- A-face-centered $\text{Bi}_{0.75}\text{Ca}_{3.25}\text{Mn}_3\text{O}_{10}$: A Bi-based orthorhombic 4310-type bilayered manganite

Physical Review B, 64, (2001), pp. 172405

Y.L. Qin, J.L. García-Muñoz, H.W. Zandbergen and M.T. Casais

31.- Oxygen-induced grain boundary effects on magnetotransport properties of $\text{Sr}_2\text{FeMoO}_6+d$

Physical Review B, 64, (2001), pp. 180406(R)

D. Niebieskikwiat, A. Caneiro, R.D. Sánchez and J. Fontcuberta

32.- Magnetic Structure of the HoNiO_3 perovskite

Physical Review B, 64, pp. 144417-1

M.T. Fernández-Díaz, J.A. Alonso, M.J. Martínez-Lope, M.T. Casais and J.L. García-Muñoz

33.- Magnetic and magnetotransport properties of $\text{GdBaCo}_2\text{O}_{5+d}$: A high magnetic-field study

Physical Review B, 64, (2001), pp. 214401

M. Respaud, C. Frontera, J.L. García-Muñoz, M.A.G. Aranda, B. Raquet, J.M. Broto, H. Rakoto, M. Goiran, A. Llobet and J. Rodríguez-Carvajal

34.- Alternating current susceptibility study of the low doped regime of $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ perovskites

Journal of Applied Physics, 89 (11), (2001), pp. 6633-6635

B. Martínez, V. Laukhin, J. Fontcuberta, J. Nogués, V. Skumryev, J.S. Muñoz, L. Pinsard and A. Revcolevschi

35.- Magneto-optical Kerr effect in laser-patterned $\text{La}_{2/3}\text{Sr}_{1/3}\text{MnO}_3$ epitaxial thin films

Journal of Applied Physics, 89 (11), (2001), pp. 6958-6960

M. Bibes, D. Hrabovsky, B. Martínez, A.R. Fert, V. Trtík, M. Varela and J. Fontcuberta

36.- Thickness dependence of surface roughness and transport properties of $\text{La}_{2/3}\text{Ca}_{1/3}\text{MnO}_3$ epitaxial thin films

Journal of Applied Physics, 89 (11), (2001), pp. 6686-6688

M. Bibes, Ll. Balcells, S. Valencia, S. Sena, B. Martínez, J. Fontcuberta, S. Nadolski, M. Wojcik and E. Jedryka

37.- Paramagnetic susceptibility and ferromagnetism in $\text{Sr}_2\text{FeMoO}_6$ perovskites

Journal of Applied Physics, 89 (11), (2001), pp. 7684-7686

J. Navarro, Ll. Balcells, B. Martínez and J. Fontcuberta

38.- Unconventional magnetic behavior of iron-oxide nanoparticles in polymeric matrices

Journal of Applied Physics, 90 (3), (2001), pp. 1534-1539