

Articles in journals, 2005

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

B.- MAGNETIC MATERIALS

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D.- INORGANIC, ORGANOMETALLIC MATERIALS, AND COORDINATION COMPOUNDS

E.- ORGANIC MATERIALS

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

G.- NOT INCLUDED IN JCR (JOURNAL CITATION REPORTS)

- 1.- M. Kaczmarek, O.N. Bedoya-Martinez and E.R. Hernandez
Phase diagram of silicon from atomistic simulations
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- 2.- H.A. Al-Britthen, R. Yang, M.B. Haider, C. Constantin, E. Lu, A.R. Smith, N. Sandler and P. Ordejón
Scanning tunnelling microscopy and surface simulation of Zinc-Blende GaN(001) intrinsic 4X reconstruction: Linear gallium tetramers?
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- 3.- R. Rurali, N. Lorente and P. Ordejón
Comment on "Molecular distortions and chemical bonding of a large π -conjugated molecule on a metal surface"
Physical Review Letters, 95, (2005), pp. 209601-1
- 4.- B. Braïda, S. Adams and E. Canadell
Concerning the structure of hydrogen molybdenum bronze phase III. A combined theoretical-experimental study
Chemistry of Materials, 17, (2005), pp. 5957-5969
- 5.- P. Alemany, M. Llunell and E. Canadell
Electronic structure of Li_2Ga and Li_9Al_4 , two solids containing infinite and uniform zigzag chains
Inorganic Chemistry, 44, (2005), pp. 374-381
- 6.- P. Alemany, M. Llunell and E. Canadell
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- 7.- E. Machado, M. Kaczmarek, P. Ordejón, D. Garg, J. Norman and H. Cheng
First-principles analyses and predictions on the reactivity of barrier layers of Ta and TaN toward organometallic precursors for deposition of copper films
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- 8.- C. Herdes, M.A. Santos, F. Medina and L.F. Vega
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- 10.- J. Hernández-Cobos, H. Saint-Martin, A.D. Mackie, L.F. Vega and I. Ortega-Blake
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- 11.- A. Olivet, D. Duque and L.F. Vega
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Journal of Chemical Physics, 123 (19), (2005), pp. 194508-1 - 194508-8
- 12.- M. Machón, S. Reich, H. Telg, J. Maulzsch, P. Ordejón and C. Thomsen
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Physical Review B, 71, (2005), pp. 035416-1 - 035416-4
- 13.- D. Errandonea, A. Segura, F.J. Manjón, A. Chevy, E. Machado, G. Tobias, P. Ordejón and E. Canadell
Crystal symmetry and pressure effects on the valence band structure of γ -InSe and ϵ -GaSe: Transport measurements and electronic structure calculations
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- 14.- K. Trachenko, J.M. Pruneda, E. Artacho and M.T. Dove
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- 15.- T. Yildirim, J. Íñiguez and S. Ciraci
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- 24.- A.M.A. Dias, C.M.B. Gonçalves, A.I. Caço, L.M.N.B.F. Santos, M.M. Piñeiro, L.F. Vega, J.A.P. Coutinho and I.M. Marrucho
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B.- MAGNETIC MATERIALS

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