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**CIENCIA, TECNOLOGÍA E
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TRANSFORMAR LA SOCIEDAD**

No	ARTICLES	AUTHORS	PUBLICATION	REGISTERED USER AT CNS	USER'S INSTITUTIONAL AFFILIATION
1	Emergence of collective motion in a model of interacting Brownian particles	c. Couder-Castañeda, H. Barrios-Piña, I. Gitler, M. Arroyo	Journal Physical Review Letters	Dr. Victor Dossetti	Benemérita Universidad Autónoma de Puebla
2	Realistic artificial DNA sequences as negative controls for computational genomics	Juan Caballero, Arian F. A. Smit, Leory Hood and Gustavo Glusman	Nucleic Acid Research, 2014, Vol. 42, No. 12 e99	Dr. Juan Caballero	Universidad Autónoma de Querétaro
3	Adsorption and Diffusion of Hydrogen on C60-Supported Pt _n Clusters	R. Mendez-Camacho and R.A. Guirado Lopez	The Journal Ph. Ch. C 2013, 117, 10059-10069	Dr. Ricardo Guirado	Universidad Autónoma de San Luis Potosí
4	Thiol based molecular overlayers absorbed on C60: Role of the end-group and charge state on the stability of the complexes	R. Chavira and R. A. Guirado-Lopez	The Journal of Chemical Physics 139, 174307 (2013)	Dr. Ricardo Guirado	Universidad Autónoma de San Luis Potosí
5	Atomics charges of Cl-ions confined in a model Escherichia coli CIC-Cl-/H ⁺ ion exchanger: a density functional theory study	P.G Nieto-Delgado, J. Arreola and R.A. Guirado-Lopez	Molecular Ph: An international Jou. at the Interface Between Ch. and Ph., 2013	Dr. Ricardo Guirado	Universidad Autónoma de San Luis Potosí
6	Structural electronic properties, and aggregation behavior of hydroxylated carbon nanotubes	A.B. Lopez-Oyama, R.A. Silva Molina, J. Ruiz-Garcia, R. Gamez-Corrales and R.A. Guirado Lopez	The Journal of Chemical Physics 141, 2014	Dr. Ricardo Guirado	Universidad Autónoma de San Luis Potosí
7	First-principles calculations of the indigo encapsulation and absorption by MgO nanotubes	F. Sanchez-Ochoa, Gregorio H. Cocoltzi, Gabriel I. Canto and Noboru Takeuchi	Journal of Applied Physics 115, 2014	Dr. Gregorio Hernández	Benemérita Universidad Autónoma de Puebla
8	Detection of Paracetamol by Armchair BN Nanotubes: A Molecular study	E. Chigo Anota, Gregorio H. Cocoltzi, J.F. Sanchez Ramirez, A. Bautista Hernandez	Structural Chemistry 25 (2014) 895	Dr. Alejandro Bautista	Benemérita Universidad Autónoma de Puebla
9	Theoretical study on small clusters of BaTiO ₃ using DFT calculations	M. Salazar-Villanueva, A. Bautista Hernandez, E. Chigo Anota, J.I. Rodriguez Mora, J.A. Ascensio and A. Macias Cervantes	Molecular Simulation 39 (2013) 545	Dr. Alejandro Bautista	Benemérita Universidad Autónoma de Puebla
10	Structural and Vibrational Stability of M and Z phases of Silicon and Germanium from first principles	A. Bautista-Hernandez, T. Rangel, A.H. Romero, G.-M. Rignanese, M. Salazar Villanueva, E. Chigo-Anota	Journal of Applied Physics 113 (2013) 193504	Dr. Alejandro Bautista	Benemérita Universidad Autónoma de Puebla
11	A performance study of Dual Xeon Phi cluster for the forward modeling of gravitational fields.	Maricela Arroyo, Carlos Couder-Castañeda, Alfredo Trujillo-Alcantara, Nain Vera-Chavez and Israel-Enrique Herrera-Díaz	Cluster computing manuscript No.	Dra. Maricela Arroyo	Centro de Investigación y de Estudios Avanzados

12	Performance of a Code Migration for the Simulation of Supersonic Ejector Flow to SMP, MIC, and GPU Using OpenMP, OpenMP+LEO, and OpenACC Directives	C. Couder-Castañeda, H. Barrios-Piña, I. Gitler, M. Arroyo	Hindawi Publishing Corporation Scientific Programming Volume 2015, Article ID 739107, 20 pages	Dra. Maricela Arroyo	Centro de Investigación y de Estudios Avanzados
13	The effect of the supramolecular network of (Z)-3-(4-(dyphenylamino)phenoxy)-2-pyridin-2-yl)-acrylonitrile on the fluorescence behavior of a single crystal: Experimental and theoretical studies	M. Judith Percino, Margarita Ceron, Guillermo Soriano-Moro, M. Eugenia Castro, Victor M. Chapela, Jose Bonilla, Marisol Reyes-Reyes and Roman Lopez-Sandoval	The Royal Society of Chemistry 2014	Dr. Roman Lopez	Instituto Potosino de Investigación Científica y Tecnológica A.C.
14	Switching the charge delocalization in Boron-doped carbon nanoribbons to elucidate the dibenzothiophene absorption	Pablo Navarro-Santos, Pablo Lopez-Albarran, and J.L. Ricardo-Chavez	-	Dr. Ricardo Chavez	Instituto Potosino de Investigación Científica y Tecnológica A.C.
15	Conformational landscape of an immunoglobulin domain explored by molecular dynamics	Nina Pastor Colon and D. Alejandro Fernandez Velasco	Mensaje Bioquímico, Vol. XXXV (2011)	Dra. Carmen Pastor	Universidad Autónoma del Estado de México
16	Noncollinear spin-fluctuation theory of transition-metal magnetism: Role of transverse spin fluctuations in Fe	R. Garibay-Alonso, J. Dorantes-Dávila y G. M. Pastor	American Physical Society B 91, 184408 (2015)	R. Garibay-Alonso	Universidad Autónoma del Estado de México
17	Finite temperature orbital and spin magnetism of small Fe linear chains	R. Garibay-Alonso, I. Guillén-Escamilla, M. Reyes-Reyes y R. López-Sandoval	J. Phys.: Condens. Matter 27 (2015) 286001 (10pp)	R. Garibay-Alonso	Universidad de Guadalajara
18	Propiedades Magnéticas y Catalíticas de Nanoaleaciones Metálicas	Dr. José Luis Ricardo Chávez, M.C. Ana Paulina Ponce Tadeo, M.C. Peter Ludwig Rodríguez Kessier	-	Dr. José Luis Ricardo Chávez	Instituto Potosino de Investigación Científica y Tecnológica
19	Magnetismo no colineal en películas delgadas de hierro depositadas sobre cobre	Dr. Raúl Garibay Alonso	-	Dr. Raúl Garibay Alonso	Universidad de Guadalajara
20	Ab initio simulation of p-type silicon crystals	E.R.L. Loustau, J.A. del Río, J. Tagüeña-Martínez, L.E. Sansores, R. Nava, M.B. de la Mora	Solid State Communications 152, 1619-1624 (2012)	E.R.L. Loustau	Universidad Nacional Autónoma de México
21	Conformational landscape of an immunoglobulin domain explored by molecular dynamics.	Nina Pastor Colón, D. Alejandro Fernández Velasco	Mensaje Bioquímico, Vol. XXXV, 2011, 53-66.	Nina Pastor Colón	Universidad Autónoma del Estado de Morelos
22	Cell-based and in-silico studies on the high intrinsic activity of two boron-containing salbutamol derivatives at	Marvin A. Soriano-Ursúa, Daniel A. McNaught-Flores, Gustavo Nieto-Alamilla, Aldo Segura-	Bioorganic & Medicinal Chemistry 20 (2012) 933-941	Aldo Segura-Cabrera	Instituto Politécnico Nacional

	the human b2-adrenoceptor	Cabrera, José Correa-Basurto, José A. Arias-Montaño, José G. Trujillo-Ferrara.			
23	A computational analysis of the binding mode of closantel as inhibitor of the Onchocerca volvulus chitinase: insights on macrofilaricidal drug design	Aldo Segura-Cabrera, Virgilio Bocanegra-García, Cristian Lizarazo-Ortega, Xianwu Guo, Jose Correa-Basurto, Mario A. Rodríguez-Perez	J Comput Aided Mol Des. 2011 Dec;25(12):1107-19	Aldo Segura-Cabrera	Instituto Politécnico Nacional
24	Tuning the electronic properties of armchair carbon nanoribbons by a selective boron doping	P Navarro-Santos, J L Ricardo-Chávez, M Reyes-Reyes, J L Rivera and R López-Sandoval	Journal of Physics Condensed Matter 22(50):505302 · December 2010 (9pp)	J L Ricardo-Chávez	Instituto Potosino de Investigación y Científica y Tecnológica
25	Specific heat of Sb: Isotopic and spin-orbit effects from measurements and ab initio calculations	Serrano, J. Kremer, R. K. Cardona, M. Siegle, G. Díaz-Sánchez, L. E. Romero, A. H.	J. Serrano, R. K. Kremer, M. Cardona, G. Siegle, L.E. Díaz-Sánchez and A.H. Romero Specific heat of Sb: Isotopic and spin-orbit effects from measurements and ab initio calculations. Phys. Rev. B 77 054303 (2008)	Dr. Aldo Romero	Centro De Investigación. Y de Estudios Avanzados Del Instituto Politécnico Nacional
26	The mesoscale variability in the Caribbean Sea. Part 2: Energy sources	Julien Jouanno, Julio Sheinbauma, Bernard Barnier, Jean-Marc Molines	Jouanno, J., J. Sheinbaum Pardo, B. Barnier y J. M. Molines. (2009) The mesoscale variability in the Caribbean Sea. Part. II: Energy sources. Ocean Modelling. 26(3-4): 226-239 p. (PA: 90723)	-	-
27	Influencia del cobreen la adsorción de hidrógeno en celdas de grafeno	Juan Salvador Arellano Peraza	-	-	-
28	Algunas Configuraciones del equilibrio para átomos de hidrógeno contenidos en una celda de grafeno III	Juan Salvador Arellano Peraza	-	-	-
29	Numerical Study of the effect of the environmental temperature in the natural two-dimensional convection of heat in grain stored at cylindrical silos.	M. Calderón-Ramírez, M. Carrera-Rodríguez, G.M. Martínez-González, J.L., Navarrete-Bolaños, J.E. Botello-Álvarez, R.Rico-Martínez y H. Jiménez-Islas	Rev. Mex. Ing. Quím vol.8 no. 1 México abr. 2009 pp. 77-91	-	-
30	Parallel Approach for Time Series Analysis with General Regression Neural Networks	Cuevas-Tello, J.C., González-Grimaldo, R.A., Rodríguez-González, O., Pérez-González, H.G., Vital-Ochoa, O. (2012)	Journal of Applied Reserach Research and Technology, 2(10), pp. 162-179	J.C. Cuevas-Tello	Universidad Autónoma de San Luis Potosí

31	Computo Evolutivo y Supercómputo	J.C. Cuevas-Tello	-	J.C. Cuevas Tello	Universidad Autónoma de San Luis Potosí
32	Electronic spin-fluctuation theory of finite-temperature cluster magnetism: Size and environment dependence in FeN	R.Garibay-Alonso, J. Dorantes-Dávila, and G.M. Pastor	Phys. Rev. B 79, 134401 Published 3 April 2009	Dr. Raúl Garibay Alonso	Universidad Autónoma del Estado de Coahuila
33	Functional-integral study of spin fluctuations in small Fe clusters	R. Garibay-Alonso, J. Dorantes-Dávila, and G. M. Pastor	THE EUROPEAN PHYSICAL JOURNAL D 52, 167-170 (2009)	Dr. Raúl Garibay Alonso	Universidad de Guadalajara
34	Differential, state-to-state, and total-charge-transfer cross sections for H ⁺ colliding with Ar	R. Cabrera-Trujillo, A. Amaya-Tapia, and A. Antillón	Phys. Rev. A 79, 012712-Published 26 January 2009	-	-
35	Onset of non-collinear magnetism in small Fe clusters	P.Ruíz-Díaz, J. Dorantes-Dávila, G.M Pastor	Eur. Phys. J.D 52, 175-178 (2009)	Dr. Jesús Dorantes Dávila	Universidad Autónoma de San Luis Potosí
36	Laser and isotope effects in charge transfer processes in atomic collisions	R. Cabrera-Trujillo	Radiation Effects & Defects in Solids Vol. 164, Nos. 7-8, July-August 2009, 402-408	-	-
37	Spin-reorientation transitions in cobalt nanowires: Role of the microstructure and finite-size effects.	R.A. Guirado-López, J.M. Montejano-Carrizalez, and J.L. Morán-López	Phys. Rev. B 77, 134431- Published 16 April 2008	Dr. Ricardo Guirado	Universidad Autónoma de San Luis Potosí
38	First principles study of anatase and rutile Ti=2 doped with Eu ions: a comparison of GGA and LDA+U calculations	Rubio-Ponce, A. Conde-Gallardo and D. Olguín	Phys. Rev. B 78, 035107-Published 9 July 2008	-	-
39	Lattice Properties of PbX (X=S, Se, Te): Experimental Studies and ab initio Calculations Including Spin-Orbit Effects	A.H. Romero, M. Cardona, R.K. Kremer, R. Lauck, G. Siegle, J. Serrano, X.C. Gonze	Phys. Rev. B 78, 224302- Published 2 December 2008	Dr. Aldo H. Romero	Instituto Politécnico Nacional
40	Effect of sulphur doping on manganese clusters: an ab initio study	J. Mejía-López, J. Pinto, A. H. Romero	Eur. Phys. J.D 50, 45-52 (2008)	Dr. Aldo H. Romero	Instituto Politécnico Nacional
41	Quantum electronic transport through supported Si ₂₉ H ₂₄ clusters on an ideal Si [111] surface	Samuel E. Baltazar, Mario De Menech, Ulf Saalman, Aldo H. Romero and Martín E. García	Journal of Applied Physics Dr. Aldo H. Romero 103, 023714 (2008)	Dr. Aldo H. Romero	Instituto Politécnico Nacional
42	A two dimensional Heusler alloy model	R. Rodríguez-Albaa, F. Aguilera-Granjab, J.L. Morán-López	Solid State Communications 149 (2009) 73-77	-	-
43	Influence of S and P Doping in a Graphene Sheet	A.L.E. García1_x0001_, S.E. Baltazar, A.H. Romero, J.F. Pérez Robles, and A. Rubio3	Journal of Computational and Theoretical Nanoscience, Volume 5, Number 11, November 2008, pp. 2221-2229 (9)	Dr. Aldo Romero	Instituto Politécnico Nacional
44	Comparative ab initio study of the structural, electronic, and magnetic trends of isoelectronic	F. Aguilera-Granja, A.García-Fuente, and A. Vega	Phys. Rev. B 78, 134425-Published 29 October 2008	-	-

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45	Modifying the endohedral La-ion location in both neutral and positively charged polyhydroxylated metallofullerenes	J.G. Rodríguez-Zavala, I. Padilla-Osuna, and R.A. Guirado-López	Phys. Rev. B 78, 155426-Published 24 October 2008	Dr. Ricardo Guirado	Universidad Autónoma de San Luis Potosí
46	Understanding the elusive magnetic behaviour of manganese clusters	José Mejía-López, Aldo H. Romero, Martín E. García, and J.L. Morán-López	Phys. Rev. B 78, 134405-Published 6 October 2008	Dr. Aldo Romero	Instituto Politécnico Nacional
47	Recent developments in magnetic nanostructures	J.L. Morán-López, R.A. Guirado-López, J.M. Montejano-Carrizalez, F. Aguilera-Granja, R. Rodríguez-Alba	CURRENT SCIENCE, VOL.95, NO. 9, 10 NOVEMBER 2008	Dr. Ricardo Guirado	Universidad Autónoma de San Luis Potosí
48	Bimetallic Fe-Ni Cluster Alloys: Stability of Core (Fe)-Shell(Ni) Arrays and Their Role Played in the Structure and Magnetic behavior	R.A. Guirado-López and F. Aguilera-Granja	Phys. Chem. C112, 6729 (2008).	Dr. Ricardo Guirado	Universidad Autónoma de San Luis Potosí
49	Lattice dynamics of wurtzite and rocksalt AlN under high pressure: Effect of compression on the crystal anisotropy of wurtzite-type semiconductors	Francisco Javier Manjón, Daniel Errandonea, Aldo Humberto Romero, Núria Garro, Jorge Serrano, Martín Kuball	Phys. Rev. B 77.205204-Published 16 May 2008	Dr. Aldo Romero	Centro de Investigación y de Estudios avanzados del Instituto Politécnico Nacional
50	The mesoscale variability in the Caribbean Sea. Part 1: Simulations and characteristics with an embedded model	Julien Jouannoa, Julio Sheinbauma, Bernard Barnier, Jean—Marc Molines, Laurent Debreuc, Florian Lemariéc	Ocean Modelling, Elsevier, 2008, 23 (3-4), pp. 82-101	-	-
51	Heat capacity of PbS: Isotope effects	M. Cardona, R.K. Kremer, R. Lauck, G. Siegle, J.Serrano, A.H. Romero	Phys. Rev. B 76, 075211-Published 31 August 2007	Dr. Aldo Romero	Centro de Investigación y de Estudios avanzados del Instituto Politécnico Nacional
52	A density-functional study of the structures, binding energies and magnetic moments of the clusters Mo _N (N= 2-13), Mo ₁₂ Fe, Mo ₁₂ Co and Mo ₁₂ Ni	F Aguilera-Granja, A Vega and L J Gallego	Nanotechnology, Volume 19, Number 14 Published 5 March 2008	-	-
53	Estudio de las propiedades electrónicas de cúmulos de Pd: un estudio comparativo usando distintas técnicas y aproximaciones	J. Ferrer, F. Aguilera Granja, J. M. Montejano Carrizales, A. Vega, J. Rogan, G. García	Rev.mex. fis. Vol. 54 no.2 149-161 México abr.2008	Dr. Juan Martín Montejano	Universidad Autónoma de San Luis Potosí
54	Effect of the Spin-Orbit Interaction on the thermodynamic Properties of Crystals: Specific Heat of Bismuth	Díaz-Luis, A.H. Romero, M. Cardona, R.K. Kremer, X. Gonze	Physical Review Letters 99 (16): 165504 October 2007	Dr. Aldo Romero	Centro de Investigación y de Estudios avanzados del Instituto Politécnico Nacional