Escuela de Pregrado – Facultad de Ciencias – Universidad de Chile

Nombres:

PATRICIO ARMANDO

Apellidos:

FUENTEALBA ROSAS

Título Profesional o Grado Académico (incluya el año de obtención):

LICENCIADO EN FISICA, 1978, UNIVERSIDAD DE CHILE

Estudios de Postgrado o Especialización (institución donde lo obtuvo y año de obtención):

PHD. EN FÍSICA, UNIVERSIDAD DE STUTTGART, ALEMANIA, 1984

Actividad Actual e Institución en la cual trabaja:

PROFESOR TITULAR DE LA UNIVERSIDAD DE CHILE, DEPARTAMENTO DE FÍSICA, FACULTAD DE CIENCIAS.

Reseña de su actividad laboral actual:

Área de Investigación: Física Atómica y Molecular.

Línea de Investigación: Su preocupación es el estudio de la estructura electrónica de la materia, átomos, moléculas, clusters y sólidos. Básicamente se desenvuelve en dos líneas de investigación: Aplicaciones de la Teoría del Funcional de la Densidad a Reactividad en Química y el estudio de la estructura electrónica de clusters atómicos. A través de cálculos teóricos, el Profesor Fuentealba trata de predecir algunas de las propiedades de los cluster: saber si son estables o no, si es que es posible encontrarlas, aislarlas, entre otros.

PUBICACIONES INDEXADAS:

1.

Title: Ab Initio Molecular Dynamics Simulations of Ti2 on C20 Collisions and C20Ti2 Configurations Author(s): Muñoz, Francisco; Cardenas, Carlos; Rogan, José; et al. Source: **The Journal of Physical Chemistry C** Volume: **117** Issue: **8** Pages: **4287-**

4291 Published:**2013/02/28** DOI: **10.1021/jp3120786** / Author-provided URL : added 30-Apr-13

2.

Title: A new isomer of C-20 and a way to a new C-240
Author(s): Cardenas, Carlos; Munoz, Francisco; Munoz, Macarena; et al.
Source: **Physical Chemistry Chemical Physics** Volume: **14** Issue: **43** Pages: **14810-14814** Published:**2012** Times Cited: **1** DOI: **10.1039/c2cp41691c** added30-Apr-13

3.

Title: A Computationally Efficient and Reliable Bond Order Measure Author(s): Mera-Adasme, R; Mendizabal, F; Olea-Azar, C; et al.
Source: **Journal of Physical Chemistry a** Volume: **115** Issue: **17** Pages: **4397-4405** Published: **MAY 5 2011** Times Cited: **2** DOI: **10.1021/jp107498h** added12-Jul-11

4.

Title: Assembling Small Silicon Clusters Using Criteria of Maximum Matching of the Fukui Functions Author(s): Osorio, Edison; Ferraro, Marta B.; Ona, Ofelia B.; et al.
Source: **Journal of Chemical Theory and Computation** Volume: **7** Issue: **12** Pages: **3995-4001** Published:**2011**
Times Cited: **1** DOI: **10.1021/ct200643z** added02-Apr-12

5.

Title: Big Bang Methodology Applied to Atomic Clusters Author(s): Centeno, J; Fuentealba, P. Source: **International Journal of Quantum Chemistry** Volume: **111** Issue: **7-8** Pages: **1419-1435**Published: **JUN-JUL 2011**
Times Cited: **2** DOI: **10.1002/qua.22860** added12-Jul-11

6.

Title: Electron Localization Function as a Measure of Electron Delocalization and Aromaticity
Author(s): Fuentealba, Patricio; Santos, Juan C.
Source: **Current Organic Chemistry** Volume: **15** Issue: **20** Pages: **3619-3626** Published: **2011** Times Cited: **2** added02-Apr-12

7.

Title: Exploration of the (Ethanol)(4)-Water Heteropentamers Potential Energy Surface by Simulated Annealing and Ab Initio Molecular Dynamics
Author(s): Mejia, Sol M.; Orrego, Juan F.; Espinal, Juan F.; et al.
Source: **International Journal of Quantum Chemistry** Volume: **111** Issue: **12** Pages: **3080-3096**Published: **2011**
Times Cited: **1** DOI: **10.1002/qua.22664** added02-Apr-12

8.

Title: Octahedral complexes of the series of actinides hexafluorides AnF(6)
Author(s): Perez-Villa, A; David, J; Fuentealba, P; et al.
Source: **Chemical Physics Letters** Volume: **507** Issue: **1-3** Pages: **57-62** Published: **2011**
Times Cited: **5** DOI: **10.1016/j.cplett.2011.03.064** added08-Jul-11

9.

Title: The Fukui Potential and the Capacity of Charge and the Global Hardness of Atoms
Author(s): Cardenas, Carlos; Tiznado, William; Ayers, Paul W.; et al.
Source: **Journal of Physical Chemistry A** Volume: **115** Issue: **11** Pages: **2325-2331** Published: **2011**
Times Cited: **8** DOI: **10.1021/jp109955q** added02-Apr-12

10.

Title: Density functional based reactivity parameters: Thermodynamic or kinetic concepts?
Author(s): Fuentealba, P; David, J; Guerra, D
Source: **Journal of Molecular Structure-Theochem** Volume: **943** Issue: **1-**

3 Pages: **127-137** Published:**2010**
Times Cited: **4** DOI: **10.1016/j.theochem.2009.11.014** added08-Jul-11

11.

Title: Theoretical characterization of SOME amides and esters DERIVATIVES of valproic acid
Author(s): Comelli, NC; Fuentealba, P; Castro, EA; et al.
Source: **Journal of Molecular Modeling** Volume: **16** Issue: **2** Pages: **343-359** Published: **2010**
Times Cited: **0** DOI: **10.1007/s00894-009-0554-6** added08-Jul-11

12.

Title: Topological Analysis of the Fukui Function
Author(s): Fuentealba, P; Florez, E; Tiznado, W
Source: **Journal of Chemical Theory and Computation** Volume: **6** Issue: **5** Pages: **1470-1478** Published:**MAY 2010**
Times Cited: **13** DOI: **10.1021/ct100022w** added12-Jul-11

13.

Title: A Theoretical Study of Alkali Metal Atomic Clusters: From Li-n to Cs-n (n=2-8)
Author(s): Florez, E; Fuentealba, P
Source: **International Journal of Quantum Chemistry** Volume: **109** Issue: **5** Pages: **1080-1093** Published:**APR 2009**
Times Cited: **7** DOI: **10.1002/qua.21906** added12-Jul-11

14.

Title: Chemical Reactivity Descriptors for Ambiphilic Reagents: Dual Descriptor, Local Hypersoftness, and Electrostatic Potential
Author(s): Cardenas, C; Rabi, N; Ayers, PW; et al.
Source: **Journal of Physical Chemistry a** Volume: **113** Issue: **30** Pages: **8660-8667** Published: **JUL 30 2009**
Times Cited: **25** DOI: **10.1021/jp902792n** added12-Jul-11

15.

Title: Density-functional theory with additional basic variables: Extended Legendre transform
Author(s): Ayers, PW; Fuentealba, P
Source: **Physical Review a** Volume: **80** Issue: **3** Published: **SEP 2009**
Times Cited: **17** DOI: **10.1103/PhysRevA.80.032510** added12-Jul-11

16.

Title: Endohedral Cluster of Li10O with T-d Symmetry
Author(s): Centeno, J; Contreras, R; Fuentealba, P
Source: **Journal of Physical Chemistry a** Volume: **113** Issue: **48** Pages: **13451-13456** Published: **2009**
Times Cited: **2** DOI: **10.1021/jp902665p** added08-Jul-11

17.

Title: Modeling Pressure Effects on the Electronic Properties of Ca, Sr, and Ba by the Confined Atoms Model
Author(s): Guerra, D; Vargas, R; Fuentealba, P; et al.
Source: **Advances in Quantum Chemistry, Vol 58** Volume: **58** Pages: **1-12** Published: **2009**
Times Cited: **2** DOI: **10.1016/S0065-3276(09)00705-9** added08-Jul-11

18.

Title: On the Gas-Phase Electronic Chemical Potential of Anions
Author(s): Perez-Mendez, C; Fuentealba, P; Contreras, R
Source: **Journal of Chemical Theory and Computation** Volume: **5** Issue: **11** Pages: **2944-2949** Published:**2009**
Times Cited: **2** DOI: **10.1021/ct900164a** added08-Jul-11

19.

Title: On the Nucleophilicity of Boryllithium Compounds. A Theoretical Study
Author(s): Jaramillo, P; Perez, P; Fuentealba, P
Source: **Journal of Physical Chemistry a** Volume: **113** Issue: **24** Pages: **6812-6817** Published: **2009**
Times Cited: **8** DOI: **10.1021/jp900945k** added08-Jul-11

20.

Title: On the Principle of Spin Potential Equalization
Author(s): Guerra, D; Contreras, R; Cedillo, A; et al.
Source: **Journal of Physical Chemistry a** Volume: **113** Issue: **7** Pages: **1390-1396** Published: **2009**
Times Cited: **2** DOI: **10.1021/jp8066348** added08-Jul-11

21.

Title: Solvent Effects on Global Reactivity Properties for Neutral and Charged Systems Using the Sequential Monte Carlo Quantum Mechanics Model
Author(s): Jaramillo, P; Perez, P; Fuentealba, P; et al.
Source: **Journal of Physical Chemistry B** Volume: **113** Issue: **13** Pages: **4314-4322** Published: **2009**
Times Cited: **11** DOI: **10.1021/jp808210y** added08-Jul-11

22.

Title: Theoretical Study of the Structure and Electronic Properties of Si3On- and Si6On- (n=1-6) Clusters. Fragmentation and Formation Patterns
Author(s): Tiznado, W; Ona, OB; Caputo, MC; et al.
Source: **Journal of Chemical Theory and Computation** Volume: **5** Issue: **9** Pages: **2265-2273** Published:**SEP 2009**
Times Cited: **5** DOI: **10.1021/ct900320r** added12-Jul-11

23.

Title: Chemical reactivity of oxygen vacancies on the MgO surface: Reactions with CO2, NO2 and metals
Author(s): Florez, E; Fuentealba, P; Mondragon, F
Source: **Catalysis Today** Volume: **133** Pages: **216-222** Published: **APR-JUN 2008**
Times Cited: **14** DOI: **10.1016/j.cattod.2007.12.087** added 12-Jul-11**24.**

Title: Effect of surface site on the spin state of first-row transition metals adsorbed on MgO: Embedded cluster model and hybrid density functional theory calculations
Author(s): Florez, E; Mondragon, F; Fuentealba, P; et al.
Source: **Physical Review B** Volume: **78** Issue: **7** Published: **AUG 2008**
Times Cited: **6** DOI: **10.1103/PhysRevB.78.075426** added12-Jul-11

25.

Title: Relationship between the electrophilicity and sigma(p) Hammett constant in Baeyer-Villiger reactions
Author(s): Meneses, L; Araya, A; Pilaquinga, F; et al.
Source: **Chemical Physics Letters** Volume: **460** Issue: **1-3** Pages: **27-30** Published: **2008**
Times Cited: **14** DOI: **10.1016/j.cplett.2008.05.044** added08-Jul-11

26.

Title: Relativistic effects on the hexafluorides of group 10 metals
Author(s): David, J; Fuentealba, P; Restrepo, A
Source: **Chemical Physics Letters** Volume: **457** Issue: **1-3** Pages: **42-44** Published: **2008**
Times Cited: **10** DOI: **10.1016/j.cplett.2008.04.003** added08-Jul-11

27.

Title: Stochastic search of the quantum conformational space of small lithium and bimetallic lithium-sodium clusters
Author(s): Perez, JF; Florez, E; Hadad, CZ; et al.

Source: **Journal of Physical Chemistry a** Volume: **112** Issue: **25** Pages: **5749-5755** Published: **2008**
Times Cited: **16** DOI: **10.1021/jp802176w** added08-Jul-11

28.

Title: Theoretical ro-vibrational spectrum of CF+
Author(s): Inostroza, N; Letelier, JR; Senent, ML; et al.
Source: **Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy** Volume: **71** Issue: **3**Pages: **798-802** Published: **2008**
Times Cited: **2** DOI: **10.1016/j.saa.2008.02.027** added08-Jul-11

29.

Title: Theoretical study of the surface reactivity of alkaline earth oxides: Local density of states evaluation of the local softness
Author(s): Cardenas, C; De Proft, F; Chamorro, E; et al.
Source: **Journal of Chemical Physics** Volume: **128** Issue: **3** Published: **2008**
Times Cited: **9** DOI: **10.1063/1.2819239** added08-Jul-11

30.

Title: Aromaticity and electronic structure of silabenzenes. Possible existence of a new cluster Si6Li6
Author(s): Santos, JC; Fuentealba, P
Source: **Chemical Physics Letters** Volume: **443** Issue: **4-6** Pages: **439-442** Published: **AUG 6 2007**
Times Cited: **24** DOI: **10.1016/j.cplett.2007.06.105** added12-Jul-11

31.

Title: beta-Scission of thioimidoyl radicals (R-1-N-C-center dot=S-R-2): A theoretical scale of radical leaving group ability
Author(s): Guerra, D; Fuentealba, P; Aizman, A; et al.
Source: **Chemical Physics Letters** Volume: **443** Issue: **4-6** Pages: **383-388** Published: **AUG 6 2007**
Times Cited: **5** DOI: **10.1016/j.cplett.2007.06.053** added08-Jul-11

32.

Title: Density functional theory characterization of the formation of copper clusters on F-s and F-s(+) centers on a MgO surface
Author(s): Florez, E; Mondragon, F; Truong, TN; et al.
Source: **Surface Science** Volume: **601** Issue: **3** Pages: **656-664** Published: **FEB 1 2007**
Times Cited: **5** DOI: **10.1016/j.susc.2006.10.040** added12-Jul-11

33.

Title: Further exploration of the Fukui function, hardness, and other reactivity indices and its relationships within the Kohn-Sham scheme
Author(s): Fuentealba, P; Chamorro, E; Cardenas, C
Source: **International Journal of Quantum Chemistry** Volume: **107** Issue: **1** Pages: **37-45** Published: **2007**
Times Cited: **15** DOI: **10.1002/qua.21021** added08-Jul-11

34.

Title: Local hardness: An application to electrophilic additions
Author(s): Meneses, L; Araya, A; Pilaquinga, F; et al.
Source: **Chemical Physics Letters** Volume: **446** Pages: **170-175** Published: **2007**
Times Cited: **5** DOI: **10.1016/j.cplett.2007.07.092** added08-Jul-11

35.

Title: Nuclear fukui functions from nonintegral electron number calculations
Author(s): Cardenas, C; Chamorro, E; Galvan, M; et al.
Source: **International Journal of Quantum Chemistry** Volume: **107** Issue: **4** Pages: **807-815** Published:**2007**
Times Cited: **4** DOI: **10.1002/qua.21202** added08-Jul-11

36.

Title: Relationship between basicity and nucleophilicity
Author(s): Jaramillo, P; Perez, P; Fuentealba, P
Source: **Journal of Physical Organic Chemistry** Volume: **20** Issue: **12** Pages: **1050-1057** Published: **2007**
Times Cited: **18** DOI: **10.1002/poc.1251** added08-Jul-11

37.

Title: Definition of a nucleophilicity scale
Author(s): Jaramillo, P; Perez, P; Contreras, R; et al.
Source: **Journal of Physical Chemistry a** Volume: **110** Issue: **26** Pages: **8181-8187** Published: **JUL 6 2006**
Times Cited: **52** DOI: **10.1021/jp057351q** added08-Jul-11

38.

Title: Effect of Ni and Pd on the geometry, electronic properties, and active sites of copper clusters
Author(s): Florez, E; Mondragon, F; Fuentealba, P
Source: **Journal of Physical Chemistry B** Volume: **110** Issue: **28** Pages: **13793-13798** Published: **JUL 20 2006**
Times Cited: **8** DOI: **10.1021/jp060521u** added12-Jul-11

39.

Title: Experimental and theoretical study on the substitution reactions of aryl 2,4-dinitrophenyl carbonates with quinuclidines
Author(s): Castro, EA; Campodonico, PR; Contreras, R; et al.
Source: **Tetrahedron** Volume: **62** Issue: **11** Pages: **2555-2562** Published: **MAR 13 2006**
Times Cited: **30** DOI: **10.1016/j.tet.2005.12.044** added08-Jul-11

40.

Title: Hardness and softness kernels, and related indices in the spin polarized version of density functional theory
Author(s): Guerra, D; Contreras, R; Perez, P; et al.
Source: **Chemical Physics Letters** Volume: **419** Issue: **1-3** Pages: **37-43** Published: **2006**
Times Cited: **10** DOI: **10.1016/j.cplett.2005.11.039** added08-Jul-11

41.

Title: Homofugality: A new reactivity index describing the leaving group ability in homolytic substitution reactions
Author(s): Guerra, D; Castillo, R; Andres, J; et al.
Source: **Chemical Physics Letters** Volume: **424** Issue: **4-6** Pages: **437-442** Published: **JUN 24 2006**
Times Cited: **9** DOI: **10.1016/j.cplett.2006.04.092** added08-Jul-11

42.

Title: Modified genetic algorithms to model cluster structures in medium-sized silicon clusters: Si-18-Si-60
Author(s): Ona, O; Bazterra, VE; Caputo, MC; et al.
Source: **Physical Review a** Volume: **73** Issue: **5** Published: **MAY 2006**
Times Cited: **25** DOI: **10.1103/PhysRevA.73.053203** added12-Jul-11

43.

Title: Nuclear reactivity indices in the context of spin polarized density functional theory
Author(s): Cardenas, C; Lamsabhi, AM; Fuentealba, P
Source: **Chemical Physics** Volume: **322** Issue: **3** Pages: **303-310** Published: **MAR 20 2006**
Times Cited: **10** DOI: **10.1016/j.chemphys.2005.09.001** added08-Jul-11

44.

Title: Nucleophilicity scale for n- and pi-nucleophiles
Author(s): Jaramillo, P; Fuentealba, P; Perez, P
Source: **Chemical Physics Letters** Volume: **427** Issue: **4-6** Pages: **421-**

425 Published: **AUG 31 2006**
Times Cited: **23** DOI: **10.1016/j.cplett.2006.06.066** added08-Jul-11

45.
Title: On the variations of electronic chemical potential and chemical hardness induced by solvent effects
Author(s): Meneses, L; Fuentealba, P; Contreras, R
Source: **Chemical Physics Letters** Volume: **433** Issue: **1-3** Pages: **54-57** Published: **DEC 29 2006**
Times Cited: **10** DOI: **10.1016/j.cplett.2006.10.124** added08-Jul-11

46.
Title: Relationship between singlet-triplet excitation energies and the Kohn-Sham orbitals obtained with potentials that exhibit a wrong asymptotic behavior
Author(s): Vazquez-Mayagoitia, A; Vargas, R; Nichols, JA; et al.
Source: **Chemical Physics Letters** Volume: **419** Issue: **1-3** Pages: **207-212** Published: **FEB 15 2006**
Times Cited: **5** DOI: **10.1016/j.cplett.2005.11.075** added08-Jul-11

47.
Title: Structural, electronic and magnetic properties of vacancies in single-walled carbon nanotubes
Author(s): Orellana, W; Fuentealba, P
Source: **Surface Science** Volume: **600** Issue: **18** Pages: **4305-4309** Published: **2006**
Times Cited: **21** DOI: **10.1016/j.susc.2006.01.158** added08-Jul-11**48.**

Title: Transition-metal atom adsorption on an F-s defect site of MgO (100) and the interaction with a hydrogen atom
Author(s): Florez, E; Mondragon, F; Truong, TN; et al.
Source: **Physical Review B** Volume: **73** Issue: **11** Published: **MAR 2006**
Times Cited: **10** DOI: **10.1103/PhysRevB.73.115423** added12-Jul-11

49.
Title: A theoretical study on the reaction mechanism for the Bergman cyclization from the perspective of the electron localization function and catastrophe theory
Author(s): Santos, JC; Andres, J; Aizman, A; et al.
Source: **Journal of Physical Chemistry a** Volume: **109** Issue: **16** Pages: **3687-3693** Published: **APR 28 2005**
Times Cited: **28** DOI: **10.1021/jp0441947** added12-Jul-11

50.
Title: A theoretical study on the reaction mechanism for the Bergman cyclization from the perspective of the electron localization function and catastrophe theory
Author(s): Santos, JC; Andres, J; Aizman, A; et al.
Source: **Journal of Physical Chemistry a** Volume: **109** Issue: **16** Pages: **3687-3693** Published: **APR 28 2005**
Times Cited: **28** DOI: **10.1021/jp0441947**

51.
Title: An aromaticity scale based on the topological analysis of the electron localization function including sigma and pi contributions
Author(s): Santos, JC; Andres, J; Aizman, A; et al.
Source: **Journal of Chemical Theory and Computation** Volume: **1** Issue: **1** Pages: **83-86** Published: **JAN-FEB 2005**
Times Cited: **83** DOI: **10.1021/ct0499276** added12-Jul-11

52.
Title: Comparison among four different ways to condense the Fukui function
Author(s): Tiznado, W; Chamorro, E; Contreras, R; et al.
Source: **Journal of Physical Chemistry a** Volume: **109** Issue: **14** Pages: **3220-3224** Published: **APR 14 2005**
Times Cited: **33** DOI: **10.1021/jp0450787** added08-Jul-11

53.

Title: Condensation of the highest occupied molecular orbital within the electron localization function domains
Author(s): Chamorro, E; Duque, M; Cardenas, C; et al.
Source: **Journal of Chemical Sciences** Volume: **117** Issue: **5** Pages: **419-424** Published: **SEP 2005** Times Cited: **6** added08-Jul-11

54.

Title: Electronic properties of small bimetallic LinCum (n,m <= 4) clusters. A comparison with Li-n and Cu-m clusters
Author(s): Fuentealba, P; Padilla-Campos, L
Source: **International Journal of Quantum Chemistry** Volume: **102** Issue: **5** Pages: **498-505** Published:**APR 20 2005**
Times Cited: **9** DOI: **10.1002/qua.20459** added08-Jul-11

55.

Title: Pseudopotential and electron propagator methods for the calculation of the photoelectron spectra of anionic silicon clusters: Predictions on Si-10(-)
Author(s): Tiznado, WA; Fuentealba, P; Ortiz, JV
Source: **Journal of Chemical Physics** Volume: **123** Issue: **14** Published: **OCT 8 2005**
Times Cited: **3** DOI: **10.1063/1.2048506** added08-Jul-11

56.

Title: Relationship between the electrophilicity of substituting agents and substrate selectivity in Friedel-Crafts reactions
Author(s): Meneses, L; Fuentealba, P; Contreras, R
Source: **Tetrahedron** Volume: **61** Issue: **4** Pages: **831-836** Published: **JAN 24 2005**
Times Cited: **15** DOI: **10.1016/j.tet.2004.11.038** added08-Jul-11

57.

Title: Relationships between the electrophilicity index and experimental rate coefficients for the aminolysis of thiolearbonates and dithiocarbonates
Author(s): Campodonico, RR; Fuentealba, P; Castro, EA; et al.
Source: **Journal of Organic Chemistry** Volume: **70** Issue: **5** Pages: **1754-1760** Published: **MAR 4 2005**
Times Cited: **29** DOI: **10.1021/jo048127k** added08-Jul-11

58.

Title: Theoretical study of the adsorption of H on Si-n clusters, (n=3-10)
Author(s): Tiznado, W; Ona, OB; Bazterra, VE; et al.
Source: **Journal of Chemical Physics** Volume: **123** Issue: **21** Published: **DEC 1 2005**
Times Cited: **11** DOI: **10.1063/1.2128675** added08-Jul-11

59.

Title: Theoretical study of the interaction of molecular oxygen with copper clusters
Author(s): Florez, E; Tiznado, W; Mondragon, F; et al.
Source: **Journal of Physical Chemistry a** Volume: **109** Issue: **34** Pages: **7815-7821** Published: **SEP 1 2005**
Times Cited: **29** DOI: **10.1021/jp052245+** added

08-Jul-11**60.**

Title: A proposal for a new local hardness as selectivity index
Author(s): Meneses, L; Tiznado, W; Contreras, R; et al.
Source: **Chemical Physics Letters** Volume: **383** Issue: **1-2** Pages: **181-187** Published: **JAN 1 2004**
Times Cited: **34** DOI: **10.1016/j.cplett.2003.11.019** added08-Jul-11

61.

Title: Calculated geometry and paramagnetic hyperfine structure of the Cu-7 cluster
Author(s): Arratia-Perez, R; Alvarez-Thon, L; Fuentealba, P
Source: **Chemical Physics Letters** Volume: **397** Issue: **4-6** Pages: **408-**

411 Published: **OCT 21 2004**
Times Cited: **6** DOI: **10.1016/j.cplett.2004.08.139** added08-Jul-11

62.

Title: Condensation of frontier molecular orbital Fukui functions
Author(s): Bulat, FA; Chamorro, E; Fuentealba, P; et al.
Source: **Journal of Physical Chemistry a** Volume: **108** Issue: **2** Pages: **342-349** Published: **JAN 15 2004**
Times Cited: **47** DOI: **10.1021/jp036416r** added08-Jul-11

63.

Title: Local reactivity index as descriptor of benzene adsorption in cluster models of exchanged zeolite-Y
Author(s): Santos, JC; Chamorro, E; Contreras, R; et al.
Source: **Chemical Physics Letters** Volume: **383** Issue: **5-6** Pages: **612-616** Published: **JAN 15 2004**
Times Cited: **3** DOI: **10.1016/j.cplett.2003.11.083** added 08-Jul-11**64.**

Title: Modified genetic algorithms to model atomic cluster structures: CuSi clusters
Author(s): Ona, O; Bazterra, VE; Caputo, MC; et al.
Source: **Journal of Molecular Structure-Theochem** Volume: **681** Issue: **1-3** Pages: **149-155** Published:**2004**
Times Cited: **10** DOI: **10.1016/j.theochem.2004.04.060** added 08-Jul-11**65.**

Title: Modified genetic algorithms to model cluster structures in medium-size silicon clusters
Author(s): Bazterra, VE; Ona, O; Caputo, MC; et al.
Source: **Physical Review a** Volume: **69** Issue: **5** Published: **MAY 2004**
Times Cited: **17** DOI: **10.1103/PhysRevA.69.053202** added08-Jul-11

66.

Title: Sigma-pi separation of the electron localization function and aromaticity
Author(s): Santos, JC; Tiznado, W; Contreras, R; et al.
Source: **Journal of Chemical Physics** Volume: **120** Issue: **4** Pages: **1670-1673** Published: **JAN 22 2004**
Times Cited: **85** DOI: **10.1063/1.1635799** added08-Jul-11

67.

Title: The static dipole polarizability of aluminium atom: discrepancy between theory and experiment
Author(s): Fuentealba, P
Source: **Chemical Physics Letters** Volume: **397** Issue: **4-6** Pages: **459-461** Published: **OCT 21 2004**
Times Cited: **13** DOI: **10.1016/j.cplett.2004.09.013** added08-Jul-11

68.

Title: Application of the electron localization function to radical systems
Author(s): Melin, J; Fuentealba, P
Source: **International Journal of Quantum Chemistry** Volume: **92** Issue: **4** Pages: **381-390** Published:**APR 15 2003**
Times Cited: **22** DOI: **10.1002/qua.10515** added08-Jul-11

69.

Title: Chemical reactivity in the {N, N-S, nu(r)} space
Author(s): Melin, J; Aparicio, F; Galvan, M; et al.
Source: **Journal of Physical Chemistry a** Volume: **107** Issue: **19** Pages: **3831-3835** Published: **MAY 15 2003**
Times Cited: **21** DOI: **10.1021/jp034195j** added08-Jul-11

70.

Title: Correcting the atomic highest occupied orbital energy within an hybrid density functional model

Author(s): Fuentealba, P; Reyes, O
Source: **Journal of the Chilean Chemical Society** Volume: **48** Issue: **4** Pages: **115-118** Published: **DEC 2003** Times Cited: **1** added08-Jul-11

71.

Title: Electron probability distribution in AIM and ELF basins
Author(s): Chamorro, E; Fuentealba, P; Savin, A
Source: **Journal of Computational Chemistry** Volume: **24** Issue: **4** Pages: **496-504** Published: **MAR 2003**
Times Cited: **28** DOI: **10.1002/jcc.10242** added08-Jul-11

72.

Title: On the location of the electron lone pair of XeF6 and related molecules
Author(s): Simon-Manso, Y; Fuentealba, P
Source: **Journal of Molecular Structure-Theochem** Volume: **634** Pages: **89-94** Published: **SEP 5 2003**
Times Cited: **2** DOI: **10.1016/S0166-1280(03)00325-7** added08-Jul-11

73.

Title: The maximum hardness and minimum polarizability principles as the basis for the study of reaction profiles
Author(s): Gomez, B; Fuentealba, P; Contreras, R
Source: **Theoretical Chemistry Accounts** Volume: **110** Issue: **6** Pages: **421-427** Published: **2003**
Times Cited: **17** DOI: **10.1007/s00214-003-0497-4** added08-Jul-11

74.

Title: Theoretical characterization of linear [n]-ladderanes and some isomers
Author(s): Santos, JC; Fuentealba, P
Source: **Chemical Physics Letters** Volume: **377** Issue: **3-4** Pages: **449-454** Published: **AUG 15 2003**
Times Cited: **8** DOI: **10.1016/S0009-2614(03)01198-9** added08-Jul-11

75.

Title: Theoretical study of the adsorption of oxygen on a Cu(100) surface and the coadsorption with alkali atoms
Author(s): Padilla-Campos, L; Fuentealba, P
Source: **Theoretical Chemistry Accounts** Volume: **110** Issue: **6** Pages: **414-420** Published: **2003**
Times Cited: **13** DOI: **10.1007/s00214-003-0496-5** added08-Jul-11

76.

Title: Variation of the electrophilicity index along the reaction path
Author(s): Chamorro, E; Chattaraj, PK; Fuentealba, P
Source: **Journal of Physical Chemistry a** Volume: **107** Issue: **36** Pages: **7068-7072** Published: **SEP 11 2003**
Times Cited: **105** DOI: **10.1021/jp035435y**
added08-Jul-11**77.**

Title: A density functional study of the Claisen rearrangement of allyl aryl ether, allyl arylamine, allyl aryl thio ether, and a series of meta-substituted molecules through reactivity and selectivity profiles
Author(s): Gomez, B; Chattaraj, PK; Chamorro, E; et al.
Source: **Journal of Physical Chemistry a** Volume: **106** Issue: **46** Pages: **11227-11233** Published: **NOV 21 2002**
Times Cited: **19** DOI: **10.1021/jp020437o** added08-Jul-11

78.

Title: Atomic spin-density polarization index and atomic spin-density information entropy distance
Author(s): Fuentealba, P; Melin, J
Source: **International Journal of Quantum**

Chemistry Volume: **90** Issue: **1** Pages: **334-341** Published:**2002**
Times Cited: **2** DOI: **10.1002/qua.994** added08-Jul-11

79.
Title: Local reactivity index defined through the density of states describes the basicity of alkaline-exchanged zeolites
Author(s): Santos, JC; Contreras, R; Chamorro, E; et al.
Source: **Journal of Chemical Physics** Volume: **116** Issue: **10** Pages: **4311-4316** Published: **MAR 8 2002**
Times Cited: **18** DOI: **10.1063/1.1449944** added08-Jul-11

80.
Title: On the theoretical determination of the static dipole polarizability of intermediate size silicon clusters
Author(s): Bazterra, VE; Caputo, MC; Ferraro, MB; et al.
Source: **Journal of Chemical Physics** Volume: **117** Issue: **24** Pages: **11158-11165** Published: **DEC 22 2002**
Times Cited: **33** DOI: **10.1063/1.1521761** added08-Jul-11

81.
Title: The bonding nature of some simple sigmatropic transition states from the topological analysis of the electron localization function
Author(s): Chamorro, E; Santos, JC; Gomez, B; et al.
Source: **Journal of Physical Chemistry a** Volume: **106** Issue: **47** Pages: **11533-11539** Published: **NOV 28 2002**
Times Cited: **14** DOI: **10.1021/jp025958q** added08-Jul-11

82.
Title: Theoretical study of intramolecular proton transfer reactions in some thiooxalic acid derivatives
Author(s): Chamorro, E; Toro-Labbe, A; Fuentealba, P
Source: **Journal of Physical Chemistry a** Volume: **106** Issue: **15** Pages: **3891-3898** Published: **APR 18 2002**
Times Cited: **17** DOI: **10.1021/jp0143185** added08-Jul-11

83.
Title: Bonding analysis of hydrogenated lithium clusters using the electron localization function
Author(s): Fuentealba, P; Savin, A
Source: **Journal of Physical Chemistry a** Volume: **105** Issue: **51** Pages: **11531-11533** Published: **DEC 27 2001**
Times Cited: **32** DOI: **10.1021/jp012004b** added08-Jul-11

84.
Title: Higher order derivatives for nuclear indexes in the framework of density functional theory
Author(s): Chamorro, E; Fuentealba, P; Contreras, R
Source: **Journal of Chemical Physics** Volume: **115** Issue: **15** Pages: **6822-6826** Published: **OCT 15 2001** Times Cited: **10** added08-Jul-11

85.
Title: Scrutiny of the HSAB principle in some representative acid-base reactions
Author(s): Chattaraj, PK; Gomez, B; Chamorro, E; et al.
Source: **Journal of Physical Chemistry a** Volume: **105** Issue: **38** Pages: **8815-8820** Published: **2001**
Times Cited: **26** DOI: **10.1021/jp011767w** added08-Jul-11

86.
Title: Topological analysis of the electron localization function applied to the study of the [1,3] sigmatropic shift of fluorine in 3-fluorpropene
Author(s): Chamorro, E; Santos, JC; Gomez, B; et al.
Source: **Journal of Chemical Physics** Volume: **114** Issue: **1** Pages: **23-34** Published: **JAN 1 2001** Times Cited: **15** added08-Jul-11

87.

Title: Electronic structure and bonding of the ground state of alkaline-earth-metal monoxides and carbides
Author(s): Fuentealba, P; Savin, A
Source: **Journal of Physical Chemistry a** Volume: **104** Issue: **46** Pages: **10882-10886** Published: **NOV 23 2000**
Times Cited: **14** DOI: **10.1021/jp001669v** added08-Jul-11

88.

Title: Empirical energy-density relationships for the analysis of substituent effects in chemical reactivity
Author(s): Perez, P; Simon-Manso, Y; Aizman, A; et al.
Source: **Journal of the American Chemical Society** Volume: **122** Issue: **19** Pages: **4756-4762** Published:**MAY 17 2000** Times Cited: **63** added12-Jul-11

89.

Title: Molecular electronic excitations and the minimum polarizability principle
Author(s): Fuentealba, P; Simon-Manso, Y; Chattaraj, PK
Source: **Journal of Physical Chemistry a** Volume: **104** Issue: **14** Pages: **3185-3187** Published: **APR 13 2000** Times Cited: **59** added08-Jul-11**90.**

Title: On the condensed Fukui function
Author(s): Fuentealba, P; Perez, P; Contreras, R
Source: **Journal of Chemical Physics** Volume: **113** Issue: **7** Pages: **2544-2551** Published: **AUG 15 2000** Times Cited: **170** added08-Jul-11

91.

Title: Shannon entropy of 1-normalized electron density
Author(s): Fazal, SP; Sen, KD; Gutierrez, G; et al.
Source: **Indian Journal of Chemistry Section a-Inorganic Bio-Inorganic Physical Theoretical & Analytical Chemistry** Volume: **39** Issue: **1-3** Pages: **48-49** Published: **2000** Times Cited: **7** added08-Jul-11

92.

Title: Some relationships within the nonlocal (pair-site) chemical reactivity formalism of density functional theory
Author(s): Chamorro, E; Contreras, R; Fuentealba, P
Source: **Journal of Chemical Physics** Volume: **113** Issue: **24** Pages: **10861-10866** Published: **DEC 22 2000** Times Cited: **22** added08-Jul-11

93.

Title: Woodward-Hoffmann rule in the light of the principles of maximum hardness and minimum polarizability: DFT and ab initio SCF studies
Author(s): Chattaraj, PK; Fuentealba, P; Gomez, B; et al.
Source: **Journal of the American Chemical Society** Volume: **122** Issue: **2** Pages: **348-351** Published:**JAN 19 2000** Times Cited: **74** added12-Jul-11

94.

Title: A direct evaluation of regional Fukui functions in molecules
Author(s): Contreras, RR; Fuentealba, P; Galvan, M; et al.
Source: **Chemical Physics Letters** Volume: **304** Issue: **5-6** Pages: **405-413** Published: **MAY 7 1999** Times Cited: **201** added08-Jul-11

95.

Title: Basis set superposition error in atomic cluster calculations
Author(s): Fuentealba, P; Simon-Manso, Y
Source: **Chemical Physics Letters** Volume: **314** Issue: **1-2** Pages: **108-113** Published: **NOV 26 1999** Times Cited: **13** added08-Jul-11

96.

Title: Chemical bonding and reactivity: a local thermodynamic viewpoint
Author(s): Chattaraj, PK; Chamorro, E; Fuentealba, P
Source: **Chemical Physics Letters** Volume: **314** Issue: **1-2** Pages: **114-121** Published: **NOV 26 1999** Times Cited: **32** added08-Jul-11

97.

Title: Density functional study of LinHm clusters. Electric dipole polarizabilities
Author(s): Fuentealba, P; Reyes, O
Source: **Journal of Physical Chemistry a** Volume: **103** Issue: **10** Pages: **1376-1380** Published: **1999** Times Cited: **26** added08-Jul-11

98.

Title: On the ground-state structure of XBO (X = Li, Na and K) molecules
Author(s): Fuentealba, P
Source: **Chemical Physics Letters** Volume: **301** Issue: **1-2** Pages: **59-63** Published: **FEB 19 1999** Times Cited: **2** added08-Jul-11

99.

Title: The static dipole polarizability and the hardness of some new carbon hypermagnesium species
Author(s): Fuentealba, P
Source: **Journal of Molecular Structure-Theochem** Volume: **493** Pages: **139-143** Published: **1999** Times Cited: **1** added08-Jul-11

100.

Title: The variations of the hardness and the Kohn-Sham Fukui function under an external perturbation
Author(s): Fuentealba, P; Cedillo, A
Source: **Journal of Chemical Physics** Volume: **110** Issue: **20** Pages: **9807-9811** Published: **MAY 22 1999** Times Cited: **23**

101.

Title: Validity of the minimum polarizability principle in molecular vibrations and internal rotations: An ab initio SCF study
Author(s): Chattaraj, PK; Fuentealba, P; Jaque, P; et al.
Source: Journal of Physical Chemistry a Volume: 103 Issue: 46 Pages: 9307-9312 Published: NOV 18 1999 Times Cited: 87 added 08-Jul-11**102.**

Title: A modified version of the electron localization function (ELF)
Author(s): Fuentealba, P
Source: International Journal of Quantum Chemistry Volume: 69 Issue: 4 Pages: 559-565 Published:1998 Times Cited: 11 added08-Jul-11**103.**

Title: Comment on "Contribution of the shape factor sigma((r)over-right-arrow) to atomic and molecular electronegativities"
Author(s): Fuentealba, P
Source: Journal of Physical Chemistry a Volume: 102 Issue: 24 Pages: 4747-4748 Published: JUN 11 1998 Times Cited: 4 added08-Jul-11

104.

Title: On the density functional relationship between static dipole polarizability and global softness
Author(s): Simon-Manso, Y; Fuentealba, P
Source: Journal of Physical Chemistry a Volume: 102 Issue: 11 Pages: 2029-2032 Published: MAR 12 1998 Times Cited: 56 added08-Jul-11**105.**

Title: Reactivity indices and response functions in density functional theory
Author(s): Fuentealba, P
Source: Journal of Molecular Structure-Theochem Volume: 433 Pages: 113-118 Published: JUL 13 1998 Times Cited: 7 added08-Jul-11

106.

Title: Static dipole polarizabilities of small neutral carbon clusters C-n (n <= 8)
Author(s): Fuentealba, P
Source: Physical Review a Volume: 58 Issue: 5 Pages: 4232-4234 Published: NOV 1998 Times Cited: 26 added08-Jul-11

107.

Title: Calculation of the atomic kinetic energy from a density functional virial relationship
Author(s): Fuentealba, P
Source: Journal of Physics B-Atomic Molecular and Optical Physics Volume: 30 Issue: 9 Pages: 2039-2045 Published: MAY 14 1997 Times Cited: 5 added08-Jul-11

108.

Title: Modified local exchange and kinetic energy functionals for atomic systems
Author(s): Fuentealba, P
Source: Theochem-Journal of Molecular Structure Volume: 390 Pages: 1-9 Published: 1997 Times Cited: 1 added08-Jul-11

109.

Title: Static dipole polarizabilities through density functional methods
Author(s): Fuentealba, P; SimonManso, Y
Source: Journal of Physical Chemistry a Volume: 101 Issue: 23 Pages: 4231-4235 Published: JUN 5 1997 Times Cited: 28 added08-Jul-11

110.

Title: A LOCAL MODEL FOR THE HARDNESS KERNEL AND RELATED REACTIVITY PARAMETERS IN DENSITY-FUNCTIONAL THEORY
Author(s): FUENTEALBA, P
Source: Journal of Chemical Physics Volume: 103 Issue: 15 Pages: 6571-6575 Published: OCT 15 1995 Times Cited: 47 added08-Jul-11

111.

Title: FURTHER EVIDENCE OF THE CONJOINT CORRECTION TO THE LOCAL KINETIC AND EXCHANGE ENERGY DENSITY FUNCTIONALS
Author(s): FUENTEALBA, P; REYES, O
Source: Chemical Physics Letters Volume: 232 Issue: 1-2 Pages: 31-34 Published: JAN 6 1995 Times Cited: 11 added08-Jul-11

112.

Title: A CORRELATION-ENERGY FUNCTIONAL FROM A CORRELATION-FACTOR MODEL
Author(s): FUENTEALBA, P
Source: International Journal of Quantum Chemistry Volume: 49 Issue: 4 Pages: 549-557 Published:FEB 5 1994 Times Cited: 5 added08-Jul-11

113.

Title: A TEST FOR THE WILSON-LEVY CORRELATION-ENERGY FUNCTIONAL
Author(s): FUENTEALBA, P; SAVIN, A
Source: Chemical Physics Letters Volume: 217 Issue: 5-6 Pages: 566-570 Published: JAN 28 1994 Times Cited: 14 added08-Jul-11

114.

Title: ATOMIC SOFTNESS AND THE ELECTRIC-DIPOLE POLARIZABILITY
Author(s): FUENTEALBA, P; REYES, O
Source: Theochem-Journal of Molecular Structure Volume: 101 Issue: 1-2 Pages: 65-70 Published:MAY 1993 Times Cited: 0 added08-Jul-11

115.

Title: EXCHANGE ENERGY FUNCTIONAL FROM A PAULI CORRELATION-FACTOR MODEL
Author(s): FUENTEALBA, P

Source: Theochem-Journal of Molecular Structure Volume: 106 Pages: 35-38 Published: NOV 14 1993 Times Cited: 0 added08-Jul-11

116.

Title: POLARIZABILITIES AND HYPERPOLARIZABILITIES OF THE ALKALI-METAL ATOMS
Author(s): FUENTEALBA, P; REYES, O
Source: Journal of Physics B-Atomic Molecular and Optical Physics Volume: 26 Issue: 15 Pages: 2245-2250 Published: AUG 14 1993 Times Cited: 26 added08-Jul-11

117.

Title: EXCHANGE-CORRELATION FUNCTIONAL FROM A CORRELATION-FACTOR MODEL
Author(s): FUENTEALBA, P
Source: Physical Review a Volume: 45 Issue: 9 Pages: 6891-6894 Published: MAY 1 1992 Times Cited: 1 added08-Jul-11

118.

Title: HIGHER-ORDER DERIVATIVES IN DENSITY-FUNCTIONAL THEORY, ESPECIALLY THE HARDNESS DERIVATIVE DELTA-ETA/DELTA-N
Author(s): FUENTEALBA, P; PARR, RG
Source: Journal of Chemical Physics Volume: 94 Issue: 8 Pages: 5559-5564 Published: APR 15 1991 Times Cited: 91 added12-Jul-11

119.

Title: ELECTRON-AFFINITIES OF ALKALINE-EARTH-METAL ATOMS
Author(s): FUENTEALBA, P; SAVIN, A; STOLL, H; et al.
Source: Physical Review a Volume: 41 Issue: 3 Pages: 1238-1242 Published: FEB 1 1990 Times Cited: 37 added08-Jul-11

120.

Title: ELECTRON-AFFINITIES OF ALKALINE-EARTH ATOMS BY MEANS OF DIFFERENT DENSITY FUNCTIONALS
Author(s): FUENTEALBA, P; SAVIN, A; STOLL, H; et al.
Source: Physical Review a Volume: 40 Issue: 4 Pages: 2163-2165 Published: 1989 Times Cited: 9 added08-Jul-11

121.

Title: ATOMIC CORRELATION-ENERGY DIFFERENCES BY MEANS OF A POLARIZATION POTENTIAL
Author(s): FUENTEALBA, P; STOLL, H; SAVIN, A
Source: Physical Review a Volume: 38 Issue: 1 Pages: 483-486 Published: JUL 1 1988 Times Cited: 6 added08-Jul-11

122.

Title: GROUND-STATE PROPERTIES OF ALKALI AND ALKALINE-EARTH HYDRIDES
Author(s): FUENTEALBA, P; REYES, O; STOLL, H; et al.
Source: Journal of Chemical Physics Volume: 87 Issue: 9 Pages: 5338-5345 Published: NOV 1 1987 Times Cited: 63 added08-Jul-11

123.

Title: PSEUDOPOTENTIAL CALCULATIONS ON THE GROUND-STATE OF THE ALKALINE-EARTH MONOHYDRIDE IONS
Author(s): FUENTEALBA, P; REYES, O
Source: Molecular Physics Volume: 62 Issue: 6 Pages: 1291-1296 Published: DEC 20 1987 Times Cited: 18 added08-Jul-11

124.

Title: CALCULATION OF ALKALI-ION RARE-GAS POTENTIALS - THE LIHE+ ION
Author(s): FUENTEALBA, P
Source: Journal of Physics B-Atomic Molecular and Optical

Physics Volume: 19 Issue: 7 Pages: L235-L239 Published: APR 14 1986 Times Cited: 1 added08-Jul-11

125.

Title: GROUND-STATE PROPERTIES OF ALKALI DIMERS XY (X,Y=LITOCS)
Author(s): IGELMANN, G; WEDIG, U; FUENTEALBA, P; et al.
Source: Journal of Chemical Physics Volume: 84 Issue: 9 Pages: 5007-5012 Published: MAY 1 1986 Times Cited: 96 added08-Jul-11

126.

Title: PSEUDOPOTENTIAL CALCULATIONS FOR ALKALINE-EARTH ATOMS
Author(s): FUENTEALBA, P; VONSZENTPALY, L; PREUSS, H; et al.
Source: Journal of Physics B-Atomic Molecular and Optical Physics Volume: 18 Issue: 7 Pages: 1287-1296 Published: 1985 Times Cited: 149 added08-Jul-11

127.

Title: CU AND AG AS ONE-VALENCE-ELECTRON ATOMS - CI RESULTS AND QUADRUPOLE CORRECTIONS FOR CU2, AG2, CUH, AND AGH
Author(s): STOLL, H; FUENTEALBA, P; SCHWERDTFEGER, P; et al.
Source: Journal of Chemical Physics Volume: 81 Issue: 6 Pages: 2732-2736 Published: 1984 Times Cited: 67 added08-Jul-11

128.

Title: CU AND AG AS ONE-VALENCE-ELECTRON ATOMS - PSEUDOPOTENTIAL CI RESULTS FOR CUO AND AGO
Author(s): IGEL, G; WEDIG, U; DOLG, M; et al.
Source: Journal of Chemical Physics Volume: 81 Issue: 6 Pages: 2737-2740 Published: 1984 Times Cited: 31 added08-Jul-11

129.

Title: PSEUDOPOTENTIAL CALCULATIONS INCLUDING CORE-VALENCE CORRELATION - ALKALI AND NOBLE-METAL COMPOUNDS
Author(s): STOLL, H; SZENTPALY, LV; FUENTEALBA, P; et al.
Source: International Journal of Quantum Chemistry Volume: 26 Issue: 5 Pages: 725-727 Published:1984 Times Cited: 7 added08-Jul-11

130.

Title: CU AND AG AS ONE-VALENCE-ELECTRON ATOMS - PSEUDOPOTENTIAL RESULTS FOR CU-2, AG-2, CUH, AGH, AND THE CORRESPONDING CATIONS
Author(s): STOLL, H; FUENTEALBA, P; DOLG, M; et al.
Source: Journal of Chemical Physics Volume: 79 Issue: 11 Pages: 5532-5542 Published: 1983 Times Cited: 123 added08-Jul-11

131.

Title: ON THE RELIABILITY OF SEMI-EMPIRICAL PSEUDOPOTENTIALS - SIMULATION OF HARTREE-FOCK AND DIRAC-FOCK RESULTS
Author(s): FUENTEALBA, P; STOLL, H; VONSZENTPALY, L; et al.
Source: Journal of Physics B-Atomic Molecular and Optical Physics Volume: 16 Issue: 11 Pages: L323-L328 Published: 1983 Times Cited: 64 added08-Jul-11

132.

Title: PSEUDOPOTENTIAL CALCULATIONS INCLUDING CORE-VALENCE CORRELATION - ALKALI COMPOUNDS
Author(s): FUENTEALBA, P; VONSZENTPALY, L; STOLL, H; et al.
Source: Theochem-Journal of Molecular Structure Volume: 10 Pages: 213-219 Published: 1983 Times Cited: 0 added08-Jul-11

133.

Title: A PROPER ACCOUNT OF CORE-POLARIZATION WITH PSEUDOPOTENTIALS - SINGLE VALENCE-ELECTRON ALKALI COMPOUNDS
Author(s): FUENTEALBA, P; PREUSS, H; STOLL, H; et al.

Source: Chemical Physics Letters Volume: 89 Issue: 5 Pages: 418-422 Published: 1982 Times Cited: 364 added08-Jul-11

134.

Title: ON THE RELIABILITY OF SEMI-EMPIRICAL PSEUDOPOTENTIALS - DIPOLE POLARIZABILITY OF THE ALKALI ATOMS
Author(s): FUENTEALBA, P
Source: Journal of Physics B-Atomic Molecular and Optical Physics Volume: 15 Issue: 16 Pages: L555-L558 Published: 1982 Times Cited: 38 added08-Jul-11

135.

Title: PSEUDOPOTENTIAL CALCULATIONS ON RB-2+, CS-2+, RBH+, CSH+ AND THE MIXED ALKALI DIMER IONS
Author(s): VONSZENTPALY, L; FUENTEALBA, P; PREUSS, H; et al.
Source: Chemical Physics Letters Volume: 93 Issue: 6 Pages: 555-559 Published: 1982

PROYECTOS DE INVESTIGACIÓN:

INVESTIGADOR RESPONSIBLE. 1130202 EXPLORING THE DYNAMICS AND REACTIVITY OF ATOMIC AND MOLECULAR CLUSTERS. 2013
INVESTIGADOR RESPONSIBLE. 1080184 CHEMICAL REACTIVITY OF MOLECULES, CLUSTERS AND EXTENDED SYSTEMS FROM A THEORETICAL PERSPECTIVE. 2008
INVESTIGADOR RESPONSABLE. 1050294 CONCEPTOS QUIMICOS EN TEORIAS DEL FUNCIONAL DE LA DENSIDAD Y SUS APLICACIONES A MOLECULAS Y CLUSTERS. 2005
INVESTIGADOR RESPONSABLE. 1010649 APLICACIONES Y DESARROLLO DE LA TEORIA DEL FUNCIONAL DE LA DENSIDAD EN QUIMICA. 2001
INVESTIGADOR RESPONSABLE. 7010649 APLICACIONES Y DESARROLLO DE LA TEORIA DEL FUNCIONAL DE LA DENSIDAD EN QUIMICA. 2001

Actualización, mayo 2014