ABRAHAM FOUAD JALBOUT

Datos Generales

Nombre: ABRAHAM FOUAD JALBOUT

Máximo nivel de estudios: DOCTORADO

Antigüedad académica en la UNAM: 2 años

Nombramientos

Último: INVESTIGADOR TITULAR A TC No Definitivo
Instituto de Ciencias Nucleares
Desde 01-10-2008 hasta 15-08-2009

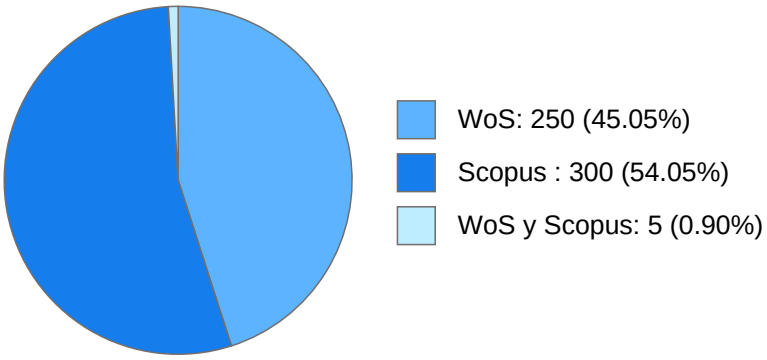
Estímulos, programas, premios y reconocimientos

SNI III 2012 - 2021
SNI II 2009 - 2011
PRIDE C - 2009

ABRAHAM FOUAD JALBOUT

DOCUMENTOS EN REVISTAS

Histórico de Documentos



#	Título	Autores	Revista	Año
1	TGA, Hirshfeld, Raman spectroscopy and computational studies of diethylammonium hexachloroplumbate [(C2H5)2NH2]2PbCl6	ABRAHAM FOUAD JALBOUT Ouasri A. El-Adel L. et al.	JOURNAL OF MOLECULAR STRUCTURE	2018
2	Metal enhanced interactions of graphene with monosaccharides	ABRAHAM FOUAD JALBOUT Pereyda-Pierre C.	CHEMICAL PHYSICS LETTERS	2016
3	Carbon nanotube surface-induced crystallization of polyethylene terephthalate (PET)	ABRAHAM FOUAD JALBOUT Cruz-Delgado, Victor J. Avila-Orta, Carlos A. et al.	Polymer	2014
4	Theoretical Study of Amino Acids Encapsulation in Zigzag Single-Walled Carbon Nanotubes	ABRAHAM FOUAD JALBOUT Chang, Chia M. Tseng, Hsiao L. et al.	JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE	2013
5	DFT study on the biomolecular storage capacity of armchair singled-walled carbon nanotubes	ABRAHAM FOUAD JALBOUT Aned de Leon Chang, Chia M. et al.	JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE	2013

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6	Theoretical design of free radical "sponges" in DNA	ABRAHAM FOUAD JALBOUT Chang, Chia M.	JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE	2013
7	New comparative theoretical calculations of some N,N-bis[(3,5-dimethylpyrazol-1-yl)methyl]phenylamines tripodal ligands	ABRAHAM FOUAD JALBOUT Bouabdallah I. Touzani R. et al.	Journal of Materials and Environmental Science	2013
8	Theoretical insights on the storage of carbon dioxide using single-walled carbon nanotubes	ABRAHAM FOUAD JALBOUT Chang, Chia M. de Leon, Aned et al.	COMPUTATIONAL MATERIALS SCIENCE	2012
9	Comparison between the two different forms of iron(IV)-oxo porphyrin and the effects of neutral axial ligand on their catalysis: A theoretical study	ABRAHAM FOUAD JALBOUT Sun, Yong Hu, Xingbang et al.	COMPUTATIONAL AND THEORETICAL CHEMISTRY	2011
10	Comparison between the two different forms of iron(IV)-oxo porphyrin and the effects of neutral axial ligand on their catalysis: A theoretical study (vol 966, pg 62, 2011)	ABRAHAM FOUAD JALBOUT Sun, Yong Hu, Xingbang et al.	COMPUTATIONAL AND THEORETICAL CHEMISTRY	2011
11	AMELIORATING THE FORMATION OF FULLERENE COMPLEXES WITH AMINO ACIDS. A THEORETICAL STUDY	ABRAHAM FOUAD JALBOUT	INTERNATIONAL JOURNAL OF MODERN PHYSICS B	2011
12	Intramolecular Hydrogen Bonding in Structural Conformers of 2-Amino Methylene Malonaldehyde: AIM and NBO Studies	ABRAHAM FOUAD JALBOUT A. de Leon Raissi, H. et al.	INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY	2010
13	Endo[Metallo] SWNT-Amino Acid Interactions: A Theoretical Study	ABRAHAM FOUAD JALBOUT	INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY	2010
14	Intramolecular Hydrogen Bond in 3-Imino-Propenylamine Isomers: AIM and NBO Studies	ABRAHAM FOUAD JALBOUT Aned de Leon Raissi, H. et al.	INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY	2010
15	[80] Fullerene-Amino Acid Interactions: Theoretical Insights	Aned de Leon ABRAHAM FOUAD JALBOUT VLADIMIR BASSIOUK EVDOKIMENKO	INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY	2010
16	Metal induced amino acid adsorption on nanotubes	ABRAHAM FOUAD JALBOUT Chang, Chia M.	Thin Solid Films	2010

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17	Glycine as a complexing agent in CdS thin films: Theoretical insights	ANED DE LEON FLORES ABRAHAM FOUAD JALBOUT Acosta-Enriquez, M. C. et al.	JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM	2010
18	The role of tautomerization in acetylacetone as a complexing agent: Theoretical perspectives	ANED DE LEON FLORES ABRAHAM FOUAD JALBOUT Acosta-Enriquez, M. C. et al.	JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM	2010
19	Nanometric layers of Cadmium Sulphide by CBD and a potential application	ABRAHAM FOUAD JALBOUT ANED DE LEON FLORES Acosta-Enriquez M.C. et al.	WSEAS Transactions on Circuits and Systems	2010
20	Theoretical Investigations of Metal-Halide Salt Encapsulated Nanotubes: A Proposal for Nano-Explosives	ABRAHAM FOUAD JALBOUT	JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE	2009
21	On the Computational Modeling of Charge Conductivity in Biopolymers	ABRAHAM FOUAD JALBOUT	JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE	2009
22	Erratum: The origin of the rotational barrier in dimethyl ether and dimethyl sulfide. a theoretical study (Journal of Theoretical and Computational Chemistry (2007) 6: 3 (421-434))	ABRAHAM FOUAD JALBOUT Jímenez-Fabian I.	J THEOR COMPUT CHEM	2009
23	Synthesis and QSAR evaluation of 2-(substituted phenyl)-1H-benzimidazoles and [2-(substituted phenyl)-benzimidazol-1-yl]-pyridin-3-yl-methanones	ABRAHAM FOUAD JALBOUT Sharma D. Narasimhan B. et al.	EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY	2009
24	The structure and stability of Si@Al12Hn (n=1-14) clusters	ABRAHAM FOUAD JALBOUT Lu Q.L. Luo Q.Q. et al.	EUROPEAN PHYSICAL JOURNAL D	2009
25	LiFePO4 as an optimum power cell material	ABRAHAM FOUAD JALBOUT Sun L.Q. Cui R.H. et al.	JOURNAL OF POWER SOURCES	2009
26	Two-center overlap integrals, three dimensional adaptive integration, and prolate ellipsoidal coordinates	ABRAHAM FOUAD JALBOUT Romanowski Z.	JOURNAL OF MATHEMATICAL CHEMISTRY	2009

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27	Novel anode Li-ion secondary batteries derived from nanocrystalline Li 4Ti5O12/polyacene materials	ABRAHAM FOUAD JALBOUT Xie H.-M. Wang R.-S. et al.	International Journal of Nanoscience	2009
28	Metallo[endo]fullerene-Amino Acid interactions. A Theoretical Study	ABRAHAM FOUAD JALBOUT	JOURNAL OF PHYSICAL CHEMISTRY C	2009
29	Computational Notes on the Analysis of C-59-Zn, C-59-Cd and C-59-Hg Fullerenes	ABRAHAM FOUAD JALBOUT A. de Leon Ibrahim, Medhat et al.	JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE	2009
30	Analysis of C-60 Doping with Gallium, Indium and Phosphorus Using Semiempirical Molecular Modelling	ABRAHAM FOUAD JALBOUT A. de Leon Ibrahim, Medhat et al.	JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE	2009
31	Monte Carlo Simulation on the RKKY Interactions of Co-Doped ZnS and ZnSe Nano-Films	ABRAHAM FOUAD JALBOUT FLAVIO FERNANDO CONTRERAS TORRES Amlan K. Roy et al.	JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE	2009
32	First-Order Transition of a Nanoscale Heteropolymer Chain with Lennard-Jones Potential	ABRAHAM FOUAD JALBOUT Aned de Leon	JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE	2009
33	Endohedral metallo [80] fullerene interactions with small polar molecules	ABRAHAM FOUAD JALBOUT	COMPUTATIONAL MATERIALS SCIENCE	2009
34	The Structures, Thermochemistry, and Electron Affinities of Hydrogenated Silicon Clusters Si6Hn/Si6Hn- (n=3-14)	ABRAHAM FOUAD JALBOUT Li, Xiao-Jun Li, Chun-Ping et al.	INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY	2009
35	Electron Localization on Molecular Surfaces by Metal Adsorption	ABRAHAM FOUAD JALBOUT THOMAS HENRY SELIGMAN SCHURCH	JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE	2009
36	Complexation of C-60 with 10-Methyl-10H-9-Chalca-10-Aza, Phospha and Arsa-Anthracene. A Theoretical Study	ABRAHAM FOUAD JALBOUT Hameed, Ali Jameel	JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE	2009

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37	Molecular Structure and Vibrational Assignment of alpha-Chloro Acetylacetone: A Density Functional Theory Study	ABRAHAM FOUAD JALBOUT M. Ali Naseri A. de Leon et al.	INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY	2009
38	Intramolecular Hydrogen Bonding in Derivatives of 3-amino-propenethial	ABRAHAM FOUAD JALBOUT M. Fazli A. de Leon et al.	INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY	2009
39	Hydrogen Bonding in Acetylacetaldehyde: Theoretical Insights from the Theory of Atoms in Molecules	ABRAHAM FOUAD JALBOUT A. de Leon Nowroozi, A. et al.	INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY	2009
40	Intramolecular Hydrogen Bonding in 3-Imino-propenylamine: Theoretical Investigations	ABRAHAM FOUAD JALBOUT A. de Leon Raissi, H. et al.	INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY	2009
41	THE ORIGIN OF THE ROTATIONAL BARRIER IN DIMETHYL ETHER AND DIMETHYL SULFIDE. A THEORETICAL STUDY (vol 6, pg 421, 2007)	I. Jimenez Fabian ABRAHAM FOUAD JALBOUT	J THEOR COMPUT CHEM	2009
42	Removal of COOH, Cd and Pb Using Water Hyacinth: FTIR and Flame Atomic Absorption Study	ABRAHAM FOUAD JALBOUT Ibrahim, M. Shaltout, A. A. et al.	J IRAN CHEM SOC	2009
43	Long-term cyclability of LiFePO4/carbon composite cathode material for lithium-ion battery applications	ABRAHAM FOUAD JALBOUT Liu, Jing Wang, Jiawei et al.	ELECTROCHIMICA ACTA	2009
44	Metalloporphyrin-Dioxygen Interactions and the Effects of Neutral Axial Ligands	ABRAHAM FOUAD JALBOUT Sun, Yong Hu, Xingbang et al.	JOURNAL OF PHYSICAL CHEMISTRY C	2009
45	Correlation analysis of the substituent electronic effects on the Mulliken charge. Resonance and field effects of substituents at para-substituted styrenyl fullerene	ABRAHAM FOUAD JALBOUT Saleh, Basil A. Essa, Ali Hashem et al.	JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM	2009
46	Adsorption of Polar Molecules on Rb/Sr@C-60. A Theoretical Analysis	ABRAHAM FOUAD JALBOUT Chang, Chia M.	JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE	2009
47	Communication on the Stability of Crystalline Silver Halide Inside Nanostructures	ABRAHAM FOUAD JALBOUT Chang, Chia M.	JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE	2009

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48	ANALYSIS OF THE INTRA-MOLECULAR HYDROGEN BOND STRENGTH IN 3-HYDROXY-PROPENETHIAL (HPT)	ABRAHAM FOUAD JALBOUT Fazli, M. Raissi, H. et al.	J THEOR COMPUT CHEM	2009
49	Prebiotic Synthesis of Simple Sugars by an Interstellar Formose Reaction	ABRAHAM FOUAD JALBOUT	ORIGINS OF LIFE AND EVOLUTION OF BIOSPHERES	2008
50	Erratum: ß-aminoacrolein: An ab initio, AIM and NBO study (International Journal of Quantum Chemestry (2008) 108 (383-390))	ABRAHAM FOUAD JALBOUT Jimenez-Fabian I. Moshfeghi E. et al.	INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY	2008
51	Synthesis, characterization, and computational study of some new organotellurium compounds containing azomethine groups	ABRAHAM FOUAD JALBOUT Al-Rubaie A.Z. Al-Masoudi W.A. et al.	HETEROATOM CHEM	2008
52	Decomposition of molecular charge speeds up the evaluation of coulomb potential	ABRAHAM FOUAD JALBOUT Romanowski Z.	ACTA PHYSICA POLONICA B	2008
53	The hydroxyacetone (CH3COCH2(OH)) torsional potential and isomerization: A theoretical study	ABRAHAM FOUAD JALBOUT FLAVIO FERNANDO CONTRERAS TORRES L. Adamowicz	INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY	2008
54	beta-aminoacrolein: An ab initio, AIM and NBO study	Isaac Jimenez Fabian ABRAHAM FOUAD JALBOUT Moshfeghi, Effat et al.	INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY	2008
55	Ammonlated solvation of excess electrons on molecular surfaces	ABRAHAM FOUAD JALBOUT	INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY	2008
56	Solvation of excess electrons trapped in charge pockets on hydrated molecular surfaces	ABRAHAM FOUAD JALBOUT FLAVIO FERNANDO CONTRERAS TORRES ROXANA MITZAYE DEL CASTILLO VAZQUEZ	INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY	2008
57	Trapping excess electrons in charge pockets on molecular surfaces in an argon matrix	ABRAHAM FOUAD JALBOUT	INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY	2008
58	Localized electron traps on extended molecular surfaces	ABRAHAM FOUAD JALBOUT	INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY	2008

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59	Density functional computational studies on the glucose and glycine Maillard reaction: Formation of the amadori rearrangement products	ABRAHAM FOUAD JALBOUT Roy, Amlan K. Shipar, Abul Haider et al.	INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY	2008
60	Formation of simple organic molecules in the interstellar medium	ABRAHAM FOUAD JALBOUT FLAVIO FERNANDO CONTRERAS TORRES Ained de Leon	INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY	2008
61	Conformational study on the structures and energies of the weakly bound complexes of AlCl3 with diatomic molecules (vol 5, pg 1007, 2007)	Isaac Jimenez Fabian ABRAHAM FOUAD JALBOUT Boutalib, Abderahim	CENT EUR J CHEM	2008
62	Low-symmetry structures of Au-32(Z) (Z =+1, 0,-1) clusters	ABRAHAM FOUAD JALBOUT FLAVIO FERNANDO CONTRERAS TORRES LUIS ANTONIO PEREZ LOPEZ et al.	JOURNAL OF PHYSICAL CHEMISTRY A	2008
63	Hydrogen sulfide stabilization of an excess electron on molecular surfaces	ABRAHAM FOUAD JALBOUT	J THEOR COMPUT CHEM	2008
64	Charge transfer stabilization of an excess electron on a molecular surface	ABRAHAM FOUAD JALBOUT Ained de Leon	INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY	2008
65	Chalcanthrene-fullerene complexes: A theoretical study	ABRAHAM FOUAD JALBOUT I. Jimenez Fabian A. de Leon et al.	JOURNAL OF ORGANOMETALLIC CHEMISTRY	2008
66	Interaction of cation-encapsulated single-walled carbon nanotubes with small polar molecules	FLAVIO FERNANDO CONTRERAS TORRES ABRAHAM FOUAD JALBOUT I. Jimenez Fabian et al.	JOURNAL OF PHYSICAL CHEMISTRY C	2008
67	Interaction of alkaline-earth metals encapsulated in SWNT with simple polar molecules	Isaac Jimenez Fabian Ained de Leon ABRAHAM FOUAD JALBOUT	JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM	2008
68	Bound state spectra of the 3D rational potential	ABRAHAM FOUAD JALBOUT Roy, Amlan K. Proynov, Emil I.	INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY	2008
69	Fullerene-amino acid interactions. A theoretical study	Ained de Leon ABRAHAM FOUAD JALBOUT VLADIMIR BASSIOUK EVDOKIMENKO	CHEMICAL PHYSICS LETTERS	2008
70	Molecular spectroscopic study of River Nile sediment in the greater Cairo region	ABRAHAM FOUAD JALBOUT Ibrahim, Medhat Hameed, Ali Jameel	APPLIED SPECTROSCOPY	2008
71	Possibility of the nonenzymatic browning (Maillard) reaction in the ISM	ABRAHAM FOUAD JALBOUT Shipar, M. Abul Haider	ORIGINS OF LIFE AND EVOLUTION OF BIOSPHERES	2008

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72	Interactions of metal-encapsulated fullerenes with solvents	ABRAHAM FOUAD JALBOUT Isaac Jimenez Fabian Aned de Leon	INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY	2008
73	Li@C-60 complexes with amino acids: A theoretical analysis	ABRAHAM FOUAD JALBOUT	JOURNAL OF ORGANOMETALLIC CHEMISTRY	2008
74	Bound states of the generalized spiked harmonic oscillator	ABRAHAM FOUAD JALBOUT Roy, Amlan K.	JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM	2008
75	Structural and theoretical studies of 4,4 '-[1,4-phenylene-bis(azanediyl)]dipent-3-en-2-one: evidence of a pi-delocalized keto-enamine	ABRAHAM FOUAD JALBOUT Benjelloun, O. T. Akkurt, M. et al.	Arkivoc	2008
76	High-rate characteristics of novel anode Li4Ti5O12/polyacene materials for Li-ion secondary batteries	ABRAHAM FOUAD JALBOUT Yu, Haiying Zhang, Xianfa et al.	ELECTROCHIMICA ACTA	2008
77	Guanine tetrad interacting with divalent metal ions (M = Fe2+, Co2+, Ni2+, Cu2+ and Zn2+): A density functional study	ABRAHAM FOUAD JALBOUT Meng, Fancui Wang, Faping et al.	JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM	2008
78	Substitution effects in biphenyl linked fullerene dimer systems	ABRAHAM FOUAD JALBOUT	JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE	2008
79	Fullerene as an electron buffer: Charge transfer and solvent interactions	Isaac Jimenez Fabian ABRAHAM FOUAD JALBOUT	JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE	2008
80	Structure and properties of a series of arylselenium [60]fulleropyrrolidine derivatives	ABRAHAM FOUAD JALBOUT FLAVIO FERNANDO CONTRERAS TORRES VLADIMIR BASSIOUK EVDOKIMENKO et al.	JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE	2008
81	Accurate calculation of the bound states of Hellmann potential	ABRAHAM FOUAD JALBOUT Roy, Amlan K. Proynov, Emil I.	JOURNAL OF MATHEMATICAL CHEMISTRY	2008
82	Structural isomers of 2-(2,3 and 4-substituted-phenyl)-1,2-benzisoselenazol-3(2H)-one: A theoretical study	ABRAHAM FOUAD JALBOUT Hameed, Ali Jameel Essa, Ali Hashem	JOURNAL OF ORGANOMETALLIC CHEMISTRY	2008

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83	The effect of substitution on the intramolecular hydrogen bonding in 3-hydroxy-propenethial	ABRAHAM FOUAD JALBOUT Raissi, H. Nasseria, M. A. et al.	INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY	2008
84	A 'Scorpion' like SWNT/carbon sheet molecular trap	Aned de Leon ABRAHAM FOUAD JALBOUT	CHEMICAL PHYSICS LETTERS	2008
85	SWNT-amino acid interactions: A theoretical study	Aned de Leon ABRAHAM FOUAD JALBOUT VLADIMIR BASSIOUK EVDOKIMENKO	CHEMICAL PHYSICS LETTERS	2008
86	Metallo[Endo]fullerene-SWNT interactions: A theoretical study	ABRAHAM FOUAD JALBOUT Aned de Leon Isaac Jimenez Fabian et al.	JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM	2008
87	The ribose and glycine Maillard reaction in the interstellar medium (ISM): A theoretical study	ABRAHAM FOUAD JALBOUT Shipar, M. D. Abul Haider	P INDIAN AS-CHEM SCI	2008
88	Effect of polyacenic semiconductors on the performance of Olivine LiFePO4	ABRAHAM FOUAD JALBOUT Yang, G. L. Xu, Y. et al.	ELECTROCHEM SOLID ST	2008
89	Structures, stabilities and tautomerizations of uracil and diphosphouracil tautomers (vol 332, pg 152, 2007)	ABRAHAM FOUAD JALBOUT Trzaskowski, B. Xia, Y. et al.	CHEMICAL PHYSICS	2008
90	Construction of novel coordination polymers with simple ligands	ABRAHAM FOUAD JALBOUT Li, Xin-Hua Hassan, Mohammad R. et al.	TRANSITION METAL CHEMISTRY	2008
91	Molecular interaction of alkanols with acrylic esters: A spectroscopic study	ABRAHAM FOUAD JALBOUT Dharmalingam, K.	JOURNAL OF MOLECULAR LIQUIDS	2008
92	Theoretical studies of 1-(4-substituted-5-hydroxymethyl-tetrahydro-furan-2-ylmethyl)-5-methyl-1H-pyrimidine-2,4-dione molecule	ABRAHAM FOUAD JALBOUT Essa, A. H.	J IRAN CHEM SOC	2008
93	Synthesis and characterization of 2,3,5,6-tetraphenylpyrazine-N,N-dioxide: New nitrone dimer species	ABRAHAM FOUAD JALBOUT Essa, Ali Hashem Al-Shamkhani, Zeki A. Nasir et al.	Heterocycles	2008
94	Structure and stability of In-X(Z) (X <= 9; Z =-1, 0, 1) clusters. Theoretical insights	ABRAHAM FOUAD JALBOUT MARIA GUADALUPE MORENO ARMENTA DONALD HOMERO GALVAN MARTINEZ et al.	CHEMICAL PHYSICS LETTERS	2008
95	Condensed extended hyper-Wiener index	ABRAHAM FOUAD JALBOUT Ji Zhi Li Xin-Hua	CHINESE J STRUC CHEM	2008

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96	Metal induced molecular nano-extraction	Ened de Leon ABRAHAM FOUAD JALBOUT	THEORETICAL CHEMISTRY ACCOUNTS	2008
97	Stabilization of Excess Electrons in Molecular Charge Pockets on Nano-Surfaces	ABRAHAM FOUAD JALBOUT Z. Romanowski F. Contrerras Torres et al.	JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE	2008
98	Nanoscale Molecular Surface Electron Solvation	ABRAHAM FOUAD JALBOUT	JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE	2008
99	Theoretical Modeling of Fullerene-Porphyrine Interactions: Computational Implications	FLAVIO FERNANDO CONTRERAS TORRES ABRAHAM FOUAD JALBOUT Oscar F. Amelines et al.	JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE	2008
100	1-(para-substituted phenyl diazenyl) Pyrrolidinofullerenes. A Theoretical Study	ABRAHAM FOUAD JALBOUT Ened de Leon Ali Hashem Essa et al.	JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE	2008
101	Structural and Electronic Properties of C60X6 (X = F, Cl, Br and I). A Theoretical Study	ABRAHAM FOUAD JALBOUT Ibrahim, Medhat Hameed, Ali Jameel et al.	JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE	2008
102	Molecular Science as an Aspiring Field for Modern Researchers in Nanotechnology	ABRAHAM FOUAD JALBOUT	JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE	2008
103	THEORETICAL STUDIES ON BOND DISSOCIATION ENERGIES FOR SOME THIOL COMPOUNDS BY DENSITRY FUNCTIONAL THEORY AND CBS-Q METHOD	ABRAHAM FOUAD JALBOUT Li Xiao-Hong Tang Zheng-Xin et al.	J THEOR COMPUT CHEM	2008
104	Interactions between cation-encapsulated single-walled carbon nanotubes M+@SWNT (M+ = H, Li, Na) and nucleophiles	FLAVIO FERNANDO CONTRERAS TORRES Oscar Amelines Sarria ABRAHAM FOUAD JALBOUT et al.	COMPUTATIONAL MATERIALS SCIENCE	2008

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105	Zigzag SWNT-amino acid interactions: Theoretical insights	Aned de Leon ABRAHAM FOUAD JALBOUT VLADIMIR BASSIOUK EVDOKIMENKO	COMPUTATIONAL MATERIALS SCIENCE	2008
106	Theoretical study of the N-NO2 bond dissociation energies for energetic materials with density functional theory	ABRAHAM FOUAD JALBOUT Li X.-H. Tang Z.-X. et al.	CHINESE J STRUC CHEM	2008
107	Theoretical study of hydrogenated Mg, Ca@ Al12 clusters	ABRAHAM FOUAD JALBOUT Lu Q.L. Luo Q.Q. et al.	JOURNAL OF CHEMICAL PHYSICS	2008
108	B3LYP theoretical calculations and structure of 4-[(2-{[(1E)-1-methyl-3-oxobutylidene]amino}ethyl)imino]pentan-2-one	ABRAHAM FOUAD JALBOUT Benjelloun O.T. Akkurt M. et al.	Arkivoc	2008
109	Self-assembly of supermolecular species directed by hydrogen bonding and aromatic p-p stacking interactions	ABRAHAM FOUAD JALBOUT Lil X.H. Xiang W.D.	ECLET QUIM	2008
110	Transformation of real spherical harmonics under rotations	ABRAHAM FOUAD JALBOUT Romanowski Z. Krukowski S.	ACTA PHYSICA POLONICA B	2008
111	Lithium-silicon Sin Li (n = 2-10) clusters and their anions: Structures, thermochemistry, and electron affinities	ABRAHAM FOUAD JALBOUT Yang J.-C. Lin L. et al.	THEORETICAL CHEMISTRY ACCOUNTS	2008
112	Toward prediction of binding affinities between the MHC protein and its peptide ligands using quantitative structure-affinity relationship approach	ABRAHAM FOUAD JALBOUT Tian F. Lv F. et al.	PROTEIN AND PEPTIDE LETTERS	2008
113	Effect of triplet encapsulated atoms in [60] fullerenes: A theoretical analysis	ABRAHAM FOUAD JALBOUT	ECLET QUIM	2008
114	Thermodynamic and kinetic approach in density functional theory studies of microscopic structure of GaN(0001) surface in ammonia-rich conditions	ABRAHAM FOUAD JALBOUT Krukowski S. Kempisty P.	JOURNAL OF CHEMICAL PHYSICS	2008
115	A DFT study of bond dissociation energies of several alkyl nitrate and nitrite compounds	ABRAHAM FOUAD JALBOUT Li X.-H. Tang Z.-X. et al.	JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM	2008
116	Structural, electronic, and magnetic properties of heterofullerene C58Si with odd number of atoms and a near planar tetracoordinate Si atom	ABRAHAM FOUAD JALBOUT Liu F.-L.	JOURNAL OF MOLECULAR GRAPHICS & MODELLING	2008
117	Overlap integrals between atomic orbitals with piecewise polynomial radial part evaluated in prolate spheroidal coordinates	ABRAHAM FOUAD JALBOUT Romanowski Z.	ACTA PHYSICA POLONICA B	2008

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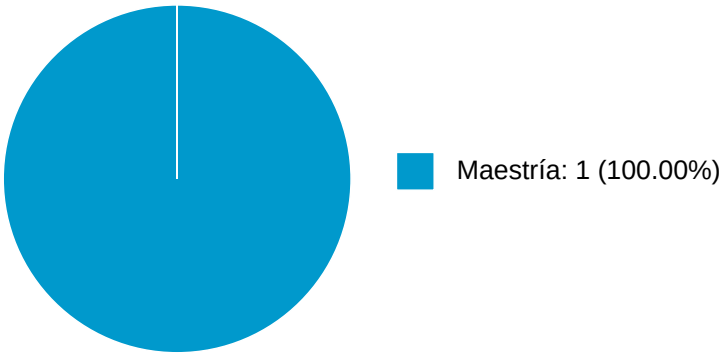

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2	Nombramientos, datos generales, estímulos, premios y reconocimientos	DGAPA	RUPA	2008-2025
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