JorgeÂ M Seminario

List of Publications by Year
in descending order

196 papers	8,253 citations	50276 46 h-index	54911 84 g-index
198 all docs	198 docs citations	198 times ranked	8123 citing authors

#	Article	IF	Citations
1	Fullerene binding effects in Al(III)/Zn(II) Porphyrin/Phthalocyanine photophysical properties and charge transport. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 269, 120740.	3.9	9
2	Li-Metal Anode in a Conventional Li-Ion Battery Electrolyte: Solid Electrolyte Interphase Formation using Ab Initio Molecular Dynamics. Journal of the Electrochemical Society, 2022, 169, 030502.	2.9	6
3	Analysis of an all-solid state nanobattery using molecular dynamics simulations under an external electric field. Physical Chemistry Chemical Physics, 2021, 23, 597-606.	2.8	16
4	Strategies towards enabling lithium metal in batteries: interphases and electrodes. Energy and Environmental Science, 2021, 14, 5289-5314.	30.8	156
5	Ion Pairing, Clustering and Transport in a LiFSI-TMP Electrolyte as Functions of Salt Concentration using Molecular Dynamics Simulations. Journal of the Electrochemical Society, 2021, 168, 040511.	2.9	14
6	CS₂ Removal from C₅ Distillates by Reactive Molecular Dynamics Simulations. Industrial & Engineering Chemistry Research, 2021, 60, 5816-5825.	3.7	4
7	Highly Reversible Aqueous Zinc Batteries enabled by Zincophilicâ€“Zincophobic Interfacial Layers and Interrupted Hydrogenâ€Bond Electrolytes. Angewandte Chemie - International Edition, 2021, 60, 18845-18851.	13.8	150
8	Highly Reversible Aqueous Zinc Batteries enabled by Zincophilicâ€“Zincophobic Interfacial Layers and Interrupted Hydrogenâ€Bond Electrolytes. Angewandte Chemie, 2021, 133, 18993-18999.	2.0	11
9	The passivity of lithium electrodes in liquid electrolytes for secondary batteries. Nature Reviews Materials, 2021, 6, 1036-1052.	48.7	201
10	Ab Initio Molecular Dynamics of Li-Metal Anode in a Phosphate-Based Electrolyte: Solid Electrolyte Interphase Evolution. Journal of the Electrochemical Society, 2021, 168, 090528.	2.9	1
11	Li-Metal Anode in Dilute Electrolyte LiFSI/TMP: Electrochemical Stability Using Ab Initio Molecular Dynamics. Journal of Physical Chemistry C, 2020, 124, 21919-21934.	3.1	19
12	Lithiation of Sulfur-Graphene Compounds Using Reactive Force-Field Molecular Dynamics Simulations. Journal of the Electrochemical Society, 2020, 167, 100555.	2.9	10
13	Solid electrolyte interphase formation between the Li_{0.29}La_{0.57}TiO₃solid-state electrolyte and a Li-metal anode: anab initiomolecular dynamics study. RSC Advances, 2020, 10, 9000-9015.	3.6	12
14	Ab Initio Study of the Interface of the Solid-State Electrolyte Li₉N₂Cl₃Âwith a Li-Metal Electrode. Journal of the Electrochemical Society, 2019, 166, A2048-A2057.	2.9	19
15	Dendrite formation in Li-metal anodes: an atomistic molecular dynamics study. RSC Advances, 2019, 9, 27835-27848.	3.6	35
16	Sigma-holes from iso-molecular electrostatic potential surfaces. Journal of Molecular Modeling, 2019, 25, 160.	1.8	8
17	Chemical and mechanical degradation and mitigation strategies for Si anodes. Journal of Power Sources, 2019, 419, 208-218.	7.8	32
18	Localized high concentration electrolyte behavior near a lithiumâ€“metal anode surface. Journal of Materials Chemistry A, 2019, 7, 25047-25055.	10.3	81

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19	Dendrite formation in silicon anodes of lithium-ion batteries. RSC Advances, 2018, 8, 5255-5267.	3.6	55
20	Simulations of a LiF Solid Electrolyte Interphase Cracking on Silicon Anodes Using Molecular Dynamics. Journal of the Electrochemical Society, 2018, 165, A717-A730.	2.9	31
21	DFT study of nano zinc/copper voltaic cells. Journal of Molecular Modeling, 2018, 24, 103.	1.8	1
22	Molecular dynamics study of thrombin capture by aptamers TBA26 and TBA29 coupled to a DNA origami. Molecular Simulation, 2018, 44, 749-756.	2.0	11
23	Investigating the effects of vacancies on self-diffusion in silicon clusters using classical molecular dynamics. Journal of Molecular Modeling, 2018, 24, 290.	1.8	15
24	Unveiling the First Nucleation and Growth Steps of Inorganic Solid Electrolyte Interphase Components. Journal of Physical Chemistry C, 2018, 122, 25858-25868.	3.1	6
25	Applying a Nonspin-Flip Reaction Scheme to Explain for the Doublet Sulfide Oxides SMO2 Observed for the Reactions of SO2 with V(4F), Nb(6D), and Ta(4F). Journal of Nanotechnology, 2018, 2018, 1-8.	3.4	0
26	Sigma-Holes in Battery Materials Using Iso-Electrostatic Potential Surfaces. Crystals, 2018, 8, 33.	2.2	6
27	PMMA-Assisted Plasma Patterning of Graphene. Journal of Nanotechnology, 2018, 2018, 1-8.	3.4	2
28	CO₂ Capture and Separations Using MOFs: Computational and Experimental Studies. Chemical Reviews, 2017, 117, 9674-9754.	47.7	837
29	Ion Diffusivity through the Solid Electrolyte Interphase in Lithium-Ion Batteries. Journal of the Electrochemical Society, 2017, 164, E3159-E3170.	2.9	108
30	Analysis of a Li-Ion Nanobattery with Graphite Anode Using Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2017, 121, 12959-12971.	3.1	41
31	Molecular dynamics simulations of the first charge of a Li-ionâ€"Si-anode nanobattery. Journal of Molecular Modeling, 2017, 23, 120.	1.8	26
32	Lithium-Ion Model Behavior in an Ethylene Carbonate Electrolyte Using Molecular Dynamics. Journal of Physical Chemistry C, 2016, 120, 16322-16332.	3.1	83
33	Electron Transport and Electrolyte Reduction in the Solid-Electrolyte Interphase of Rechargeable Lithium Ion Batteries with Silicon Anodes. Journal of Physical Chemistry C, 2016, 120, 17978-17988.	3.1	37
34	Doping Effects in the Charge Transport of Grapheneâ€"Porphyrins. Journal of Physical Chemistry C, 2016, 120, 2013-2026.	3.1	12
35	Computational Chemistry Analysis of Hydrodesulfurization Reactions Catalyzed by Molybdenum Disulfide Nanoparticles. Journal of Physical Chemistry C, 2015, 119, 29157-29170.	3.1	21
36	Structure and Reactivity of Alucone-Coated Films on Si and Li_xSi_y Surfaces. ACS Applied Materials & Interfaces, 2015, 7, 11948-11955.	8.0	39

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37	Electron Transport in Graphene-Based Nanosensors for Eu(III) Detection. Journal of Physical Chemistry C, 2015, 119, 12037-12046.	3.1	6
38	Europium Effect on the Electron Transport in Graphene Ribbons. Journal of Physical Chemistry C, 2015, 119, 22486-22495.	3.1	6
39	Formation and Growth Mechanisms of Solid-Electrolyte Interphase Layers in Rechargeable Batteries. Chemistry of Materials, 2015, 27, 7990-8000.	6.7	225
40	Density functional theory and molecular dynamics study of the uranyl ion (UO2)2+. Journal of Molecular Modeling, 2014, 20, 2150.	1.8	12
41	Ab Initio Analysis of Silicon Nano-Clusters. Journal of Physical Chemistry C, 2014, 118, 1397-1406.	3.1	12
42	Argon-Beam-Induced Defects in a Silica-Supported Single-Walled Carbon Nanotube. Journal of Physical Chemistry C, 2014, 118, 28299-28307.	3.1	8
43	Metal-Ion Effects on the Polarization of Metal-Bound Water and Infrared Vibrational Modes of the Coordinated Metal Center of Mycobacterium tuberculosis Pyrazinamidase via Quantum Mechanical Calculations. Journal of Physical Chemistry B, 2014, 118, 10065-10075.	2.6	20
44	A Quantum Chemistry Approach for the Design and Analysis of Nanosensors for Fissile Materials. Challenges and Advances in Computational Chemistry and Physics, 2014, , 1-29.	0.6	1
45	Functionalized Graphene and Cobalt Phthalocyanine Based Materials with Potential Use for Electrical Conduction. Challenges and Advances in Computational Chemistry and Physics, 2014, , 185-215.	0.6	1
46	Degradation of polyvinyl alcohol under mechanothermal stretching. Journal of Molecular Modeling, 2013, 19, 3245-3253.	1.8	12
47	Effects of trimethylaluminium and tetrakis(ethylmethylamino) hafnium in the early stages of the atomic-layer-deposition of aluminum oxide and hafnium oxide on hydroxylated GaN nanoclusters. Journal of Molecular Modeling, 2013, 19, 4419-4432.	1.8	2
48	Computational design of a CNT carrier for a high affinity bispecific anti-HER2 antibody based on trastuzumab and pertuzumab Fabs. Journal of Molecular Modeling, 2013, 19, 2797-2810.	1.8	7
49	Electron Transport Properties through Graphene Oxideâ€“Cobalt Phthalocyanine Complexes. Journal of Physical Chemistry C, 2013, 117, 23664-23675.	3.1	22
50	Design of Nanosensors for Fissile Materials in Nuclear Waste Water. Journal of Physical Chemistry C, 2013, 117, 24033-24041.	3.1	22
51	Coupling of mechanical and electronic properties of carbon nanotubes. Journal of Molecular Modeling, 2013, 19, 5237-5244.	1.8	10
52	Calculating the Hydrodynamic Volume of Poly(ethylene oxylated) Single-Walled Carbon Nanotubes and Hydrophilic Carbon Clusters. Journal of Physical Chemistry B, 2013, 117, 343-354.	2.6	23
53	Paper-based photoelectrical devices. Journal of Intelligent Material Systems and Structures, 2013, 24, 2255-2261.	2.5	13
54	Assembly of a Noncovalent DNA Junction on Graphene Sheets and Electron Transport Characteristics. Journal of Physical Chemistry C, 2013, 117, 26441-26453.	3.1	24

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55	ZnOâ€“Cellulose Composite for UV Sensing. IEEE Sensors Journal, 2013, 13, 1301-1306.	4.7	28
56	Structure and energetics of small iron clusters. Journal of Molecular Modeling, 2012, 18, 4043-4052.	1.8	33
57	Ab Initio Analysis of the Interactions of GaN Clusters with Oxygen and Water. Journal of Physical Chemistry C, 2012, 116, 12079-12092.	3.1	7
58	Molecular Dynamics Simulations of Ion-Bombarded Graphene. Journal of Physical Chemistry C, 2012, 116, 4044-4049.	3.1	47
59	Graphene-Based Vibronic Devices. Journal of Physical Chemistry C, 2012, 116, 8409-8416.	3.1	15
60	Harmonic force field for nitro compounds. Journal of Molecular Modeling, 2012, 18, 2805-2811.	1.8	3
61	Self-assembly of DNA on a gapped carbon nanotube. Journal of Molecular Modeling, 2012, 18, 3291-3300.	1.8	7
62	Molecular electrostatic potentials of DNA baseâ€“base pairing and mispairing. Journal of Molecular Modeling, 2012, 18, 91-101.	1.8	23
63	Ab Initio Analysis and Harmonic Force Fields of Gallium Nitride Nanoclusters. Journal of Physical Chemistry C, 2011, 115, 6467-6477.	3.1	16
64	DNAâ^'CNT Interactions and Gating Mechanism Using MD and DFT. Journal of Physical Chemistry C, 2011, 115, 3466-3474.	3.1	27
65	Graphene Signal Mixer for Sensing Applications. Journal of Physical Chemistry C, 2011, 115, 12128-12134.	3.1	12
66	ZnOâ^'Paper Based Photoconductive UV Sensor. Journal of Physical Chemistry C, 2011, 115, 282-287.	3.1	136
67	Electrical Characteristics of Cobalt Phthalocyanine Complexes Adsorbed on Graphene. Journal of Physical Chemistry C, 2011, 115, 16052-16062.	3.1	38
68	Computational Molecular Engineering for Nanodevices and Nanosystems. , 2011, , 347-383.		0
69	Light activation of the isomerization and deprotonation of the protonated Schiff base retinal. Journal of Molecular Modeling, 2011, 17, 2539-2547.	1.8	15
70	Spectroscopic and Photophysical Studies of Chargeâ€Transfer in a Cd₈ Thiolate Cluster Complex Containing a Coordinated Nâ€Methylâ€4,4â€²â€bipyridinium Ligand. European Journal of Inorganic Chemistry, 2011, 2011, 660-665.	2.0	14
71	Synthesis, Crystal Structure, Photophysical Properties, and DFT Calculations of a Bis(tetrathia-calix[4]arene) Tetracadmium Complex. Journal of Cluster Science, 2010, 21, 867-878.	3.3	15
72	Polypeptides in alpha-helix conformation perform as diodes. Journal of Chemical Physics, 2010, 132, 065102.	3.0	35

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73	Vibronics and plasmonics based graphene sensors. Journal of Chemical Physics, 2010, 132, 125102.	3.0	91
74	Single molecule detection using graphene electrodes. Journal of Physics B: Atomic, Molecular and Optical Physics, 2010, 43, 115101.	1.5	22
75	Molecular Dynamics Simulations of Folding of Supported Graphene. Journal of Physical Chemistry C, 2010, 114, 22472-22477.	3.1	50
76	Energetics and Vibronics Analyses of the Enzymatic Coupled Electronâ€“Proton Transfer From NfsA Nitroreductase to Trinitrotoluene. IEEE Nanotechnology Magazine, 2010, 9, 543-553.	2.0	7
77	Some Recent Studies on the Local Reactivity of O2 on Pt3 Nanoislands Supported on Mono- and Bi-Metallic Backgrounds. Modern Aspects of Electrochemistry, 2010, , 203-242.	0.2	0
78	Currentâ€“voltageâ€“temperature characteristics of DNA origami. Nanotechnology, 2009, 20, 175102.	2.6	18
79	Molecular biosensor based on a coordinated iron complex. Journal of Chemical Physics, 2009, 130, 105101.	3.0	29
80	Light-Activated Molecular Conductivity in the Photoreactions of Vitamin D₃. Journal of Physical Chemistry A, 2009, 113, 6740-6744.	2.5	11
81	Switchable Molecular Conductivity. Journal of the American Chemical Society, 2009, 131, 10447-10451.	13.7	23
82	Mechanism of carbon nanotubes unzipping into graphene ribbons. Journal of Chemical Physics, 2009, 131, 031105.	3.0	107
83	Transverse Electronic Transport in Double-Stranded DNA Nucleotides. Journal of Physical Chemistry B, 2009, 113, 6230-6239.	2.6	21
84	Protonation of O2 adsorbed on a Pt3 island supported on transition metal surfaces. Journal of Chemical Physics, 2009, 131, 044709.	3.0	2
85	Analysis of Nano and Molecular Arrays of Negative Differential Resistance Devices for Sensing and Electronics. IEEE Sensors Journal, 2009, 9, 1136-1141.	4.7	6
86	DNA origami impedance measurement at room temperature. Journal of Chemical Physics, 2009, 130, 171101.	3.0	12
87	Emulation of Molecular Programmability Using Microelectronics Programmable Devices. Journal of Physical Chemistry C, 2009, 113, 16254-16258.	3.1	2
88	Reactivity of Bimetallic Nanoclusters Toward the Oxygen Reduction in Acid Medium. Topics in Applied Physics, 2009, , 509-532.	0.8	2
89	Harmonic force field for glycine oligopeptides. International Journal of Quantum Chemistry, 2008, 108, 180-188.	2.0	18
90	Effects of substituents on molecular devices. International Journal of Quantum Chemistry, 2008, 108, 1546-1554.	2.0	14

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91	Graphene Terahertz Generators for Molecular Circuits and Sensors. Journal of Physical Chemistry A, 2008, 112, 13699-13705.	2.5	67
92	Identifying Receptorâ˜Ligand Interactions through an ab Initio Approach. Journal of Physical Chemistry B, 2008, 112, 1290-1292.	2.6	9
93	Transversal Characteristics of DNA devices. , 2008, , .		2
94	A DNA Sensor for Sequencing and Mismatches Based on Electron Transport Through Watsonâ€“Crick and Non-Watsonâ€“Crick Base Pairs. IEEE Sensors Journal, 2008, 8, 803-814.	4.7	22
95	Nanomicrointerface to read molecular potentials into current-voltage based electronics. Journal of Chemical Physics, 2008, 128, 114711.	3.0	8
96	Single-Electron Transistor-Tunable Tunnel Barrier Based Non-Volatile Memory. , 2008, , .		0
97	Program for the Analysis of Molecular Arrays of Highly Nonlinear Devices. , 2008, , .		0
98	Impedance measurements on a DNA junction. Journal of Chemical Physics, 2008, 128, 201103.	3.0	10
99	Local reactivity of O2 with Pt3 on Co3Pt and related backgrounds. Journal of Chemical Physics, 2008, 128, 204701.	3.0	7
100	Chapter 4 Analysis of programmable molecular electronic systems. Theoretical and Computational Chemistry, 2007, 17, 96-140.	0.4	2
101	Molecular dynamics simulations of signal transmission through a glycine peptide chain. Journal of Chemical Physics, 2007, 127, 134708.	3.0	11
102	Biatomic substrates for bulk-molecule interfaces: The PtCo-oxygen interface. Journal of Chemical Physics, 2007, 127, 244706.	3.0	15
103	Field-induced conformational changes in bimetallic oligoaniline junctions. Physical Review A, 2007, 75, .	2.5	43
104	Conductance model of gold-molecule-silicon and carbon nanotube-molecule-silicon junctions. Physical Review B, 2007, 76, .	3.2	15
105	Transfer of signatures from the vibrational spectrum of benzene to a silicon complex. Physical Review A, 2007, 75, .	2.5	1
106	Chapter 1 Metalâ€”moleculeâ€”semiconductor junctions:An ab initio analysis. Theoretical and Computational Chemistry, 2007, 17, 1-54.	0.4	1
107	STUDY OF NANO-STRUCTURED SILICON-PHENYL NANOCLUSTERS TOWARDS SINGLE MOLECULE SENSING. International Journal of High Speed Electronics and Systems, 2007, 17, 327-338.	0.7	3
108	Chapter 1 Electrical characteristics of bulk-molecule interfaces. Theoretical and Computational Chemistry, 2007, 18, 1-33.	0.4	0

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109	Electronic and structural properties of oligophenylene ethynylenes on Au(111) surfaces. Journal of Chemical Physics, 2007, 126, 184706.	3.0	8
110	Ab initioanalysis of electron currents through benzene, naphthalene, and anthracene nanojunctions. Nanotechnology, 2007, 18, 485701.	2.6	19
111	Molecular Dynamics Simulations of the Vibrational Signature Transfer from a Glycine Peptide Chain to Nanosized Gold Clusters. Journal of Physical Chemistry C, 2007, 111, 8366-8371.	3.1	16
112	Ab Initio Analysis of Electron Transport in Oligoglycines. Journal of Physical Chemistry C, 2007, 111, 14552-14559.	3.1	16
113	Simple Energy Corrections for Precise Atomization Energies of CHON Molecules. Journal of Physical Chemistry A, 2007, 111, 11160-11165.	2.5	6
114	Determination of precise harmonic force constants for alanine polypeptides. Computational and Theoretical Chemistry, 2007, 818, 125-129.	1.5	11
115	Electron transport in Nano-Gold-Silicon interfaces. International Journal of Quantum Chemistry, 2007, 107, 440-450.	2.0	34
116	Cascade configuration of logical gates processing information encoded in molecular potentials. International Journal of Quantum Chemistry, 2007, 107, 754-761.	2.0	14
117	Adsorption and Dissociation of H2O2on Pt and Ptâ^'Alloy Clusters and Surfaces. Journal of Physical Chemistry B, 2006, 110, 17452-17459.	2.6	76
118	The Nanocell: A Chemically Assembled Molecular Electronic Circuit. IEEE Sensors Journal, 2006, 6, 1614-1626.	4.7	31
119	Energy Correctors for Accurate Prediction of Molecular Energies. Journal of Physical Chemistry A, 2006, 110, 1060-1064.	2.5	16
120	Molecular Electrostatic Potential Devices on Graphite and Silicon Surfaces. Journal of Physical Chemistry A, 2006, 110, 12298-12302.	2.5	11
121	Platinum Testbeds:â€‰ Interaction with Oxygen. Journal of Physical Chemistry A, 2006, 110, 11968-11974.	2.5	9
122	Perfluorobutane Sulfonic Acid Hydration and Interactions with O2Adsorbed on Pt3. Journal of Physical Chemistry A, 2006, 110, 4574-4581.	2.5	12
123	Encoding Information Using Molecular Vibronics. Journal of Nanoscience and Nanotechnology, 2006, 6, 675-684.	0.9	22
124	Molecular-based processing and transfer of information in the terahertz domain for military and security applications. , 2006, , .		4
125	Moletronics modeling toward molecular potentials. International Journal of Quantum Chemistry, 2006, 106, 1964-1969.	2.0	16
126	Intensity enhancement of the vibrational spectrum of oxygen when attached to a platinum nanocluster. Journal of Chemical Physics, 2006, 125, 174302.	3.0	1

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127	MIXED-VALENCE TRANSITION METAL COMPLEX BASED INTEGRAL ARCHITECTURE FOR MOLECULAR COMPUTING (I): ATTACHMENT OF LINKER MOLECULE TO SILICON (100) - 2Ã—1 SURFACE. International Journal of High Speed Electronics and Systems, 2006, 16, 705-712.	0.7	10
128	TERAHERTZ SIGNAL TRANSMISSION IN MOLECULAR SYSTEMS. International Journal of High Speed Electronics and Systems, 2006, 16, 669-675.	0.7	15
129	Approaching reality. Nature Materials, 2005, 4, 111-113.	27.5	79
130	Ab initio analysis of electron currents in thioalkanes. International Journal of Quantum Chemistry, 2005, 102, 711-723.	2.0	79
131	Vibrational Study of a Molecular Device Using Molecular Dynamics Simulations. Journal of Nanoscience and Nanotechnology, 2005, 5, 484-495.	0.9	14
132	Electronic Structure and Electron Transport Characteristics of a Cobalt Complex. Journal of Physical Chemistry A, 2005, 109, 6628-6633.	2.5	29
133	Transmission of Vibronic Signals in Molecular Circuits. Journal of Physical Chemistry A, 2005, 109, 9712-9715.	2.5	21
134	Clustering Effects on Discontinuous Gold Film NanoCells. Journal of Nanoscience and Nanotechnology, 2004, 4, 907-917.	0.9	34
135	Negative Differential Resistance in Metallic and Semiconducting Clusters. Journal of Physical Chemistry B, 2004, 108, 6915-6918.	2.6	50
136	Nanometer-Size Conducting and Insulating Molecular Devices. Journal of Physical Chemistry B, 2004, 108, 17879-17885.	2.6	60
137	Adsorption of O, OH, and H2O on Pt-Based Bimetallic Clusters Alloyed with Co, Cr, and Ni. Journal of Physical Chemistry A, 2004, 108, 6378-6384.	2.5	80
138	A Programmable Molecular Diode Driven by Charge-Induced Conformational Changes. Journal of the American Chemical Society, 2003, 125, 14240-14241.	13.7	64
139	Theoretical Interpretation of Switching in Experiments with Single Molecules. Journal of the American Chemical Society, 2002, 124, 10266-10267.	13.7	86
140	Analysis of a dinitro-based molecular device. Journal of Chemical Physics, 2002, 116, 1671-1683.	3.0	127
141	Electron Transport through Single Molecules:Â Scattering Treatment Using Density Functional and Green Function Theories. Journal of Physical Chemistry B, 2001, 105, 471-481.	2.6	325
142	A Theoretical Analysis of Metalâ^'Molecule Contacts. Journal of the American Chemical Society, 2001, 123, 5616-5617.	13.7	205
143	Properties of Small Bimetallic Niâ^'Cu Clusters. Journal of Physical Chemistry A, 2001, 105, 7917-7925.	2.5	81
144	Theoretical Analysis of Complementary Molecular Memory Devices. Journal of Physical Chemistry A, 2001, 105, 791-795.	2.5	120

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145	Electrochemical Testing of Potential Molecular Devices. Materials Research Society Symposia Proceedings, 2000, 660, 1.	0.1	0
146	Electrochemical Testing of Potential Molecular Devices. Materials Research Society Symposia Proceedings, 2000, 636, 741.	0.1	0
147	Electrochemical Testing of Potential Molecular Devices. Materials Research Society Symposia Proceedings, 2000, 660, .	0.1	0
148	Theoretical Study of a Molecular Resonant Tunneling Diode. Journal of the American Chemical Society, 2000, 122, 3015-3020.	13.7	431
149	Lowest Energy States of Small Pd Clusters Using Density Functional Theory and Standard ab Initio Methods. A Route to Understanding Metallic Nanoprobes. Journal of Physical Chemistry A, 1999, 103, 7692-7700.	2.5	63
150	Molecular Alligator Clips for Single Molecule Electronics. Studies of Group 16 and Isonitriles Interfaced with Au Contacts. Journal of the American Chemical Society, 1999, 121, 411-416.	13.7	140
151	Molecular Currentâ^'Voltage Characteristics. Journal of Physical Chemistry A, 1999, 103, 7883-7887.	2.5	85
152	Ab initio Methods for the Study of Molecular Systems for Nanometer Technology: Toward the First-Principles Design of Molecular Computers. Annals of the New York Academy of Sciences, 1998, 852, 68-94.	3.8	15
153	Molecular Scale Electronics:Â A Synthetic/Computational Approach to Digital Computing. Journal of the American Chemical Society, 1998, 120, 8486-8493.	13.7	252
154	Use of Density Functional Methods To Compute Heats of Reactions. ACS Symposium Series, 1998, , 359-368.	0.5	1
155	Revised Structures ofN-Substituted Dibrominated Pyrrole Derivatives and Their Polymeric Products. Termaleimide Models with Low Optical Band Gaps. Journal of Organic Chemistry, 1998, 63, 2646-2655.	3.2	56
156	Theoretical Interpretation of Conductivity Measurements of a Thiotolane Sandwich. A Molecular Scale Electronic Controller. Journal of the American Chemical Society, 1998, 120, 3970-3974.	13.7	161
157	Density functional analysis of a decomposition of 4-nitro-1,2,3-triazole through the evolution of N2. International Journal of Quantum Chemistry, 1997, 61, 389-392.	2.0	31
158	Systematic study of the lowest energy states of Pd, Pd2, and Pd3. International Journal of Quantum Chemistry, 1997, 61, 515-523.	2.0	48
159	Systematic study of the lowest energy states of Aun (n=1-4) using DFT. International Journal of Quantum Chemistry, 1997, 65, 749-758.	2.0	49
160	Systematic study of the lowest energy states of Pd, Pd2, and Pd3. International Journal of Quantum Chemistry, 1997, 61, 515-523.	2.0	1
161	Calculation of intramolecular force fields from second-derivative tensors. International Journal of Quantum Chemistry, 1996, 60, 1271-1277.	2.0	231
162	Reaction energetics of tetrahedrane and other hydrocarbons: Ab initio and density functional treatments. International Journal of Quantum Chemistry, 1996, 60, 1351-1360.	2.0	3

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163	Quantitative Equilibrium Constants between CO2and Lewis Bases from FTIR Spectroscopy. The Journal of Physical Chemistry, 1996, 100, 10837-10848.	2.9	161
164	Calculation of intramolecular force fields from secondâ€derivative tensors. International Journal of Quantum Chemistry, 1996, 60, 1271-1277.	2.0	12
165	Density functional study of amine sensitization of nitromethane. Molecular Physics, 1996, 89, 1511-1520.	1.7	17
166	Molecular dynamics simulation of liquid nitromethane shocked to 143 kbar. International Journal of Quantum Chemistry, 1995, 56, 621-625.	2.0	9
167	A density functional/molecular dynamics study of the structure of liquid nitromethane. Journal of Chemical Physics, 1995, 102, 8281-8282.	3.0	56
168	Does antiaromaticity imply net destabilization?. International Journal of Quantum Chemistry, 1994, 49, 575-579.	2.0	31
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170	A study of small systems containing H and O atoms using nonlocal functionals: comparisons withab initio and experiment. International Journal of Quantum Chemistry, 1994, 52, 655-666.	2.0	19
171	Theoretical analyses of O2/H2O systems under normal and supercritical conditions. Chemical Physics Letters, 1994, 222, 25-32.	2.6	31
172	Energy changes associated with some decomposition steps of 1,3,3-trinitroazetidine. A non-local density functional study. Chemical Physics Letters, 1993, 207, 27-30.	2.6	43
173	Computational study of the structure of dinitraminic acid, HN(NO2)2, and the energetics of some possible decomposition steps. Chemical Physics Letters, 1993, 216, 348-352.	2.6	48
174	Density-Functional andab initio computational studies of palladium clusters. International Journal of Quantum Chemistry, 1993, 48, 263-268.	2.0	8
175	Some applications of local density functional theory to the calculation of reaction energetics. Theoretica Chimica Acta, 1993, 85, 127-136.	0.8	15
176	Anomalous stabilizing and destabilizing effects in some cyclic Ï€-electron systems. Canadian Journal of Chemistry, 1993, 71, 1123-1127.	1.1	24
177	C?H Bond dissociation of acetylene: Local density functional calculations. International Journal of Quantum Chemistry, 1992, 42, 267-272.	2.0	11
178	An analysis of molecular electrostatic potentials obtained by a local density functional approach. International Journal of Quantum Chemistry, 1992, 44, 113-122.	2.0	28
179	Gaussian-2 and density functional studies of H2N?NO2 dissociation, inversion, and isomerization. International Journal of Quantum Chemistry, 1992, 44, 497-504.	2.0	35
180	Calculated structures and relative stabilities of furoxan, some 1,2-dinitrosoethylenes and other isomers. Journal of Computational Chemistry, 1992, 13, 177-182.	3.3	47

#	Article	IF	Citations
181	Computational study of the concerted gas-phase triple dissociations of 1,3,5-triazacyclohexane and its 1,3,5-trinitro derivative (RDX). The Journal of Physical Chemistry, 1991, 95, 7699-7702.	2.9	49
182	Computational study of relative bond strengths and stabilities of a series of amine and nitro derivatives of triprismane and some azatriprismanes. The Journal of Physical Chemistry, 1991, 95, 1601-1605.	2.9	16
183	Energy barriers of symmetryâ€forbidden reactions: Local density functional calculations. Journal of Chemical Physics, 1991, 94, 1668-1669.	3.0	26
184	Calculation of molecular geometries and energies by a local density functional approach. International Journal of Quantum Chemistry, 1991, 40, 249-259.	2.0	24
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188	Average local ionization energies computed on the surfaces of some strained molecules. International Journal of Quantum Chemistry, 1990, 38, 645-653.	2.0	126
189	Relative bond strengths in tetrahedrane, prismane, and some of their aza analogs. Structural Chemistry, 1990, 1, 29-32.	2.0	27
190	Application ofZ-dependent perturbation theory to autoionizing states of heliumlike atoms: Feshbach projection method. Physical Review A, 1990, 42, 2562-2572.	2.5	32
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