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	CO₂ Capture and Separations Using MOFs: Computational and Experimental Studies. Chemical Reviews, 2017, 117, 9674-9754.	47.7	837
2	Theoretical Study of a Molecular Resonant Tunneling Diode. Journal of the American Chemical Society, 2000, 122, 3015-3020.	13.7	431
3	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
4	Molecular Scale Electronics:Â A Synthetic/Computational Approach to Digital Computing. Journal of the American Chemical Society, 1998, 120, 8486-8493.	13.7	252
5	Calculation of intramolecular force fields from second-derivative tensors. International Journal of Quantum Chemistry, 1996, 60, 1271-1277.	2.0	231
6	Formation and Growth Mechanisms of Solid-Electrolyte Interphase Layers in Rechargeable Batteries. Chemistry of Materials, 2015, 27, 7990-8000.	6.7	225
7	A Theoretical Analysis of Metalâ"Molecule Contacts. Journal of the American Chemical Society, 2001, 123, 5616-5617.	13.7	205
8	The passivity of lithium electrodes in liquid electrolytes for secondary batteries. Nature Reviews Materials, 2021, 6, 1036-1052.	48.7	201
9	Quantitative Equilibrium Constants between CO2and Lewis Bases from FTIR Spectroscopy. The Journal of Physical Chemistry, 1996, 100, 10837-10848.	2.9	161
10	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
11	Strategies towards enabling lithium metal in batteries: interphases and electrodes. Energy and Environmental Science, 2021, 14, 5289-5314.	30.8	156
12	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
13	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
14	ZnOâ"Paper Based Photoconductive UV Sensor. Journal of Physical Chemistry C, 2011, 115, 282-287.	3.1	136
15	Analysis of a dinitro-based molecular device. Journal of Chemical Physics, 2002, 116, 1671-1683.	3.0	127
16	Average local ionization energies computed on the surfaces of some strained molecules. International Journal of Quantum Chemistry, 1990, 38, 645-653.	2.0	126
17	Theoretical Analysis of Complementary Molecular Memory Devices. Journal of Physical Chemistry A, 2001, 105, 791-795.	2.5	120
18	Ion Diffusivity through the Solid Electrolyte Interphase in Lithium-Ion Batteries. Journal of the Electrochemical Society, 2017, 164, E3159-E3170.	2.9	108

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19	Mechanism of carbon nanotubes unzipping into graphene ribbons. Journal of Chemical Physics, 2009, 131, 031105.	3.0	107
20	Vibronics and plasmonics based graphene sensors. Journal of Chemical Physics, 2010, 132, 125102.	3.0	91
21	Theoretical Interpretation of Switching in Experiments with Single Molecules. Journal of the American Chemical Society, 2002, 124, 10266-10267.	13.7	86
22	Molecular Currentâ^'Voltage Characteristics. Journal of Physical Chemistry A, 1999, 103, 7883-7887.	2.5	85
23	Lithium-Ion Model Behavior in an Ethylene Carbonate Electrolyte Using Molecular Dynamics. Journal of Physical Chemistry C, 2016, 120, 16322-16332.	3.1	83
24	Properties of Small Bimetallic Niâ^'Cu Clusters. Journal of Physical Chemistry A, 2001, 105, 7917-7925.	2.5	81
25	Localized high concentration electrolyte behavior near a lithiumâ€“metal anode surface. Journal of Materials Chemistry A, 2019, 7, 25047-25055.	10.3	81
26	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
27	Approaching reality. Nature Materials, 2005, 4, 111-113.	27.5	79
28	Ab initio analysis of electron currents in thioalkanes. International Journal of Quantum Chemistry, 2005, 102, 711-723.	2.0	79
29	Adsorption and Dissociation of H2O2on Pt and Ptâ^'Alloy Clusters and Surfaces. Journal of Physical Chemistry B, 2006, 110, 17452-17459.	2.6	76
30	A computational study of the structures and electrostatic potentials of some azines and nitroazines. Computational and Theoretical Chemistry, 1989, 187, 95-108.	1.5	72
31	Graphene Terahertz Generators for Molecular Circuits and Sensors. Journal of Physical Chemistry A, 2008, 112, 13699-13705.	2.5	67
32	A Programmable Molecular Diode Driven by Charge-Induced Conformational Changes. Journal of the American Chemical Society, 2003, 125, 14240-14241.	13.7	64
33	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
34	Nanometer-Size Conducting and Insulating Molecular Devices. Journal of Physical Chemistry B, 2004, 108, 17879-17885.	2.6	60
35	A density functional/molecular dynamics study of the structure of liquid nitromethane. Journal of Chemical Physics, 1995, 102, 8281-8282.	3.0	56
36	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

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37	Dendrite formation in silicon anodes of lithium-ion batteries. RSC Advances, 2018, 8, 5255-5267.	3.6	55
38	A proposed interpretation of the destabilizing effect of hydroxyl groups on nitroaromatic molecules. Chemical Physics Letters, 1989, 158, 463-469.	2.6	52
39	Anomalous energy effects associated with the presence of aza nitrogens and nitro substituents in some strained systems. Computational and Theoretical Chemistry, 1990, 207, 193-200.	1.5	51
40	Negative Differential Resistance in Metallic and Semiconducting Clusters. Journal of Physical Chemistry B, 2004, 108, 6915-6918.	2.6	50
41	Molecular Dynamics Simulations of Folding of Supported Graphene. Journal of Physical Chemistry C, 2010, 114, 22472-22477.	3.1	50
42	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
43	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
44	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
45	Systematic study of the lowest energy states of Pd, Pd2, and Pd3. International Journal of Quantum Chemistry, 1997, 61, 515-523.	2.0	48
46	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
47	Molecular Dynamics Simulations of Ion-Bombarded Graphene. Journal of Physical Chemistry C, 2012, 116, 4044-4049.	3.1	47
48	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
49	Field-induced conformational changes in bimetallic oligoaniline junctions. Physical Review A, 2007, 75, .	2.5	43
50	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
51	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
52	Electrical Characteristics of Cobalt Phthalocyanine Complexes Adsorbed on Graphene. Journal of Physical Chemistry C, 2011, 115, 16052-16062.	3.1	38
53	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
54	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

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55	Polypeptides in alpha-helix conformation perform as diodes. Journal of Chemical Physics, 2010, 132, 065102.	3.0	35
56	Dendrite formation in Li-metal anodes: an atomistic molecular dynamics study. RSC Advances, 2019, 9, 27835-27848.	3.6	35
57	Clustering Effects on Discontinuous Gold Film NanoCells. Journal of Nanoscience and Nanotechnology, 2004, 4, 907-917.	0.9	34
58	Electron transport in Nano-Gold-Silicon interfaces. International Journal of Quantum Chemistry, 2007, 107, 440-450.	2.0	34
59	Anomalous energy effects in some aliphatic and alicyclic aza systems and their nitro derivatives. The Journal of Physical Chemistry, 1990, 94, 2320-2323.	2.9	33
60	Structure and energetics of small iron clusters. Journal of Molecular Modeling, 2012, 18, 4043-4052.	1.8	33
61	Computational determination of the structures and some properties of tetrahedrane, prismane, and some of their aza analogs. The Journal of Physical Chemistry, 1989, 93, 588-592.	2.9	32
62	Application ofZ-dependent perturbation theory to autoionizing states of heliumlike atoms: Feshbach projection method. Physical Review A, 1990, 42, 2562-2572.	2.5	32
63	Chemical and mechanical degradation and mitigation strategies for Si anodes. Journal of Power Sources, 2019, 419, 208-218.	7.8	32
64	Does antiaromaticity imply net destabilization?. International Journal of Quantum Chemistry, 1994, 49, 575-579.	2.0	31
65	Theoretical analyses of O2/H2O systems under normal and supercritical conditions. Chemical Physics Letters, 1994, 222, 25-32.	2.6	31
66	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
67	The Nanocell: A Chemically Assembled Molecular Electronic Circuit. IEEE Sensors Journal, 2006, 6, 1614-1626.	4.7	31
68	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
69	Electronic Structure and Electron Transport Characteristics of a Cobalt Complex. Journal of Physical Chemistry A, 2005, 109, 6628-6633.	2.5	29
70	Molecular biosensor based on a coordinated iron complex. Journal of Chemical Physics, 2009, 130, 105101.	3.0	29
71	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
72	ZnOâ€“Cellulose Composite for UV Sensing. IEEE Sensors Journal, 2013, 13, 1301-1306.	4.7	28

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73	Relative bond strengths in tetrahedrane, prismane, and some of their aza analogs. Structural Chemistry, 1990, 1, 29-32.	2.0	27
74	DNAâ˜'CNT Interactions and Gating Mechanism Using MD and DFT. Journal of Physical Chemistry C, 2011, 115, 3466-3474.	3.1	27
75	Energy barriers of symmetryâ€forbidden reactions: Local density functional calculations. Journal of Chemical Physics, 1991, 94, 1668-1669.	3.0	26
76	Molecular dynamics simulations of the first charge of a Li-ionâ€"Si-anode nanobattery. Journal of Molecular Modeling, 2017, 23, 120.	1.8	26
77	Effects of the simultaneous presence of nitro and amine substituents in cubane and some azacubanes. Structural Chemistry, 1991, 2, 153-166.	2.0	25
78	Calculation of molecular geometries and energies by a local density functional approach. International Journal of Quantum Chemistry, 1991, 40, 249-259.	2.0	24
79	Anomalous stabilizing and destabilizing effects in some cyclic Ï€-electron systems. Canadian Journal of Chemistry, 1993, 71, 1123-1127.	1.1	24
80	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
81	Switchable Molecular Conductivity. Journal of the American Chemical Society, 2009, 131, 10447-10451.	13.7	23
82	Molecular electrostatic potentials of DNA baseâ€"base pairing and mispairing. Journal of Molecular Modeling, 2012, 18, 91-101.	1.8	23
83	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
84	Encoding Information Using Molecular Vibronics. Journal of Nanoscience and Nanotechnology, 2006, 6, 675-684.	0.9	22
85	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
86	Single molecule detection using graphene electrodes. Journal of Physics B: Atomic, Molecular and Optical Physics, 2010, 43, 115101.	1.5	22
87	Electron Transport Properties through Graphene Oxideâ€"Cobalt Phthalocyanine Complexes. Journal of Physical Chemistry C, 2013, 117, 23664-23675.	3.1	22
88	Design of Nanosensors for Fissile Materials in Nuclear Waste Water. Journal of Physical Chemistry C, 2013, 117, 24033-24041.	3.1	22
89	Transmission of Vibronic Signals in Molecular Circuits. Journal of Physical Chemistry A, 2005, 109, 9712-9715.	2.5	21
90	Transverse Electronic Transport in Double-Stranded DNA Nucleotides. Journal of Physical Chemistry B, 2009, 113, 6230-6239.	2.6	21

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91	Computational Chemistry Analysis of Hydrodesulfurization Reactions Catalyzed by Molybdenum Disulfide Nanoparticles. Journal of Physical Chemistry C, 2015, 119, 29157-29170.	3.1	21
92	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
93	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
94	Ab initioanalysis of electron currents through benzene, naphthalene, and anthracene nanojunctions. Nanotechnology, 2007, 18, 485701.	2.6	19
95	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
96	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
97	Computational analysis of the structures, bond properties, and electrostatic potentials of some nitrotetrahedranes and nitroazatetrahedranes. The Journal of Physical Chemistry, 1989, 93, 4742-4745.	2.9	18
98	Harmonic force field for glycine oligopeptides. International Journal of Quantum Chemistry, 2008, 108, 180-188.	2.0	18
99	Currentâ€“voltageâ€“temperature characteristics of DNA origami. Nanotechnology, 2009, 20, 175102.	2.6	18
100	Density functional study of amine sensitization of nitromethane. Molecular Physics, 1996, 89, 1511-1520.	1.7	17
101	Calculated structures, relative energies and electrostatic potentials of some tetraaza cyclic systems. Structural Chemistry, 1990, 1, 325-332.	2.0	16
102	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
103	Energy Correctors for Accurate Prediction of Molecular Energies. Journal of Physical Chemistry A, 2006, 110, 1060-1064.	2.5	16
104	Moletronics modeling toward molecular potentials. International Journal of Quantum Chemistry, 2006, 106, 1964-1969.	2.0	16
105	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
106	Ab Initio Analysis of Electron Transport in Oligoglycines. Journal of Physical Chemistry C, 2007, 111, 14552-14559.	3.1	16
107	Ab Initio Analysis and Harmonic Force Fields of Gallium Nitride Nanoclusters. Journal of Physical Chemistry C, 2011, 115, 6467-6477.	3.1	16
108	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

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109	Some applications of local density functional theory to the calculation of reaction energetics. Theoretica Chimica Acta, 1993, 85, 127-136.	0.8	15
110	Antiaromaticity in relation to 1,3,5,7-cyclooctatetraene structures. International Journal of Quantum Chemistry, 1994, 50, 273-277.	2.0	15
111	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
112	TERAHERTZ SIGNAL TRANSMISSION IN MOLECULAR SYSTEMS. International Journal of High Speed Electronics and Systems, 2006, 16, 669-675.	0.7	15
113	Biatomic substrates for bulk-molecule interfaces: The PtCo-oxygen interface. Journal of Chemical Physics, 2007, 127, 244706.	3.0	15
114	Conductance model of gold-molecule-silicon and carbon nanotube-molecule-silicon junctions. Physical Review B, 2007, 76, .	3.2	15
115	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
116	Light activation of the isomerization and deprotonation of the protonated Schiff base retinal. Journal of Molecular Modeling, 2011, 17, 2539-2547.	1.8	15
117	Graphene-Based Vibronic Devices. Journal of Physical Chemistry C, 2012, 116, 8409-8416.	3.1	15
118	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
119	Vibrational Study of a Molecular Device Using Molecular Dynamics Simulations. Journal of Nanoscience and Nanotechnology, 2005, 5, 484-495.	0.9	14
120	Cascade configuration of logical gates processing information encoded in molecular potentials. International Journal of Quantum Chemistry, 2007, 107, 754-761.	2.0	14
121	Effects of substituents on molecular devices. International Journal of Quantum Chemistry, 2008, 108, 1546-1554.	2.0	14
122	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
123	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
124	Paper-based photoelectrical devices. Journal of Intelligent Material Systems and Structures, 2013, 24, 2255-2261.	2.5	13
125	Zâ€transition state calculations of energy changes and electrostatic potentials in isoelectronic atoms and molecules. Journal of Chemical Physics, 1989, 90, 4373-4378.	3.0	12
126	Perfluorobutane Sulfonic Acid Hydration and Interactions with O2Adsorbed on Pt3. Journal of Physical Chemistry A, 2006, 110, 4574-4581.	2.5	12

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127	DNA origami impedance measurement at room temperature. Journal of Chemical Physics, 2009, 130, 171101.	3.0	12
128	Graphene Signal Mixer for Sensing Applications. Journal of Physical Chemistry C, 2011, 115, 12128-12134.	3.1	12
129	Degradation of polyvinyl alcohol under mechanothermal stretching. Journal of Molecular Modeling, 2013, 19, 3245-3253.	1.8	12
130	Density functional theory and molecular dynamics study of the uranyl ion (UO2)2+. Journal of Molecular Modeling, 2014, 20, 2150.	1.8	12
131	Ab Initio Analysis of Silicon Nano-Clusters. Journal of Physical Chemistry C, 2014, 118, 1397-1406.	3.1	12
132	Doping Effects in the Charge Transport of Grapheneâ€“Porphyrins. Journal of Physical Chemistry C, 2016, 120, 2013-2026.	3.1	12
133	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
134	Calculation of intramolecular force fields from secondâ€derivative tensors. International Journal of Quantum Chemistry, 1996, 60, 1271-1277.	2.0	12
135	C?H Bond dissociation of acetylene: Local density functional calculations. International Journal of Quantum Chemistry, 1992, 42, 267-272.	2.0	11
136	Molecular Electrostatic Potential Devices on Graphite and Silicon Surfaces. Journal of Physical Chemistry A, 2006, 110, 12298-12302.	2.5	11
137	Molecular dynamics simulations of signal transmission through a glycine peptide chain. Journal of Chemical Physics, 2007, 127, 134708.	3.0	11
138	Determination of precise harmonic force constants for alanine polypeptides. Computational and Theoretical Chemistry, 2007, 818, 125-129.	1.5	11
139	Light-Activated Molecular Conductivity in the Photoreactions of Vitamin D₃. Journal of Physical Chemistry A, 2009, 113, 6740-6744.	2.5	11
140	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
141	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
142	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
143	Impedance measurements on a DNA junction. Journal of Chemical Physics, 2008, 128, 201103.	3.0	10
144	Coupling of mechanical and electronic properties of carbon nanotubes. Journal of Molecular Modeling, 2013, 19, 5237-5244.	1.8	10

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145	Lithiation of Sulfur-Graphene Compounds Using Reactive Force-Field Molecular Dynamics Simulations. Journal of the Electrochemical Society, 2020, 167, 100555.	2.9	10
146	Molecular dynamics simulation of liquid nitromethane shocked to 143 kbar. International Journal of Quantum Chemistry, 1995, 56, 621-625.	2.0	9
147	Platinum Testbeds:â€‰ Interaction with Oxygen. Journal of Physical Chemistry A, 2006, 110, 11968-11974.	2.5	9
148	Identifying Receptorâ˜Ligand Interactions through an ab Initio Approach. Journal of Physical Chemistry B, 2008, 112, 1290-1292.	2.6	9
149	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
150	Density-Functional andab initio computational studies of palladium clusters. International Journal of Quantum Chemistry, 1993, 48, 263-268.	2.0	8
151	Electronic and structural properties of oligophenylene ethynylenes on Au(111) surfaces. Journal of Chemical Physics, 2007, 126, 184706.	3.0	8
152	Nanomicrointerface to read molecular potentials into current-voltage based electronics. Journal of Chemical Physics, 2008, 128, 114711.	3.0	8
153	Argon-Beam-Induced Defects in a Silica-Supported Single-Walled Carbon Nanotube. Journal of Physical Chemistry C, 2014, 118, 28299-28307.	3.1	8
154	Sigma-holes from iso-molecular electrostatic potential surfaces. Journal of Molecular Modeling, 2019, 25, 160.	1.8	8
155	Local reactivity of O2 with Pt3 on Co3Pt and related backgrounds. Journal of Chemical Physics, 2008, 128, 204701.	3.0	7
156	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
157	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
158	Self-assembly of DNA on a gapped carbon nanotube. Journal of Molecular Modeling, 2012, 18, 3291-3300.	1.8	7
159	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
160	Simple Energy Corrections for Precise Atomization Energies of CHON Molecules. Journal of Physical Chemistry A, 2007, 111, 11160-11165.	2.5	6
161	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
162	Electron Transport in Graphene-Based Nanosensors for Eu(III) Detection. Journal of Physical Chemistry C, 2015, 119, 12037-12046.	3.1	6

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163	Europium Effect on the Electron Transport in Graphene Ribbons. Journal of Physical Chemistry C, 2015, 119, 22486-22495.	3.1	6
164	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
165	Sigma-Holes in Battery Materials Using Iso-Electrostatic Potential Surfaces. Crystals, 2018, 8, 33.	2.2	6
166	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
167	Molecular-based processing and transfer of information in the terahertz domain for military and security applications. , 2006, , .		4
168	CS₂ Removal from C₅ Distillates by Reactive Molecular Dynamics Simulations. Industrial & Engineering Chemistry Research, 2021, 60, 5816-5825.	3.7	4
169	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
170	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
171	Harmonic force field for nitro compounds. Journal of Molecular Modeling, 2012, 18, 2805-2811.	1.8	3
172	Chapter 4 Analysis of programmable molecular electronic systems. Theoretical and Computational Chemistry, 2007, 17, 96-140.	0.4	2
173	Transversal Characteristics of DNA devices. , 2008, , .		2
174	Protonation of O2 adsorbed on a Pt3 island supported on transition metal surfaces. Journal of Chemical Physics, 2009, 131, 044709.	3.0	2
175	Emulation of Molecular Programmability Using Microelectronics Programmable Devices. Journal of Physical Chemistry C, 2009, 113, 16254-16258.	3.1	2
176	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
177	PMMA-Assisted Plasma Patterning of Graphene. Journal of Nanotechnology, 2018, 2018, 1-8.	3.4	2
178	Reactivity of Bimetallic Nanoclusters Toward the Oxygen Reduction in Acid Medium. Topics in Applied Physics, 2009, , 509-532.	0.8	2
179	Use of Density Functional Methods To Compute Heats of Reactions. ACS Symposium Series, 1998, , 359-368.	0.5	1
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