

Vladimiro Mujica

List of Publications by Year in descending order

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135
papers

6,985
citations

61857

43
h-index

60497

81
g-index

141
all docs

141
docs citations

141
times ranked

5935
citing authors

#	ARTICLE	IF	CITATIONS
1	Theory of Chirality Induced Spin Selectivity: Progress and Challenges. <i>Advanced Materials</i> , 2022, 34, e2106629.	11.1	119
2	A Chirality-Based Quantum Leap. <i>ACS Nano</i> , 2022, 16, 4989-5035.	7.3	74
3	The contribution of intermolecular spin interactions to the London dispersion forces between chiral molecules. <i>Journal of Chemical Physics</i> , 2022, 156, .	1.2	9
4	A kinetic model for the equilibrium dynamics of absorption and scattering processes in four-wave mixing spectroscopy. <i>AIP Advances</i> , 2022, 12, 065322.	0.6	0
5	Nanoscale Phononic Analog of the Ranque-Hilsch Vortex Tube. <i>Physical Review Applied</i> , 2021, 15, .	1.5	1
6	Multiscale Thermodynamics: Energy, Entropy, and Symmetry from Atoms to Bulk Behavior. <i>Symmetry</i> , 2021, 13, 721.	1.1	7
7	Improving Seebeck coefficient of thermoelectrochemical cells by controlling ligand complexation at metal redox centers. <i>Applied Physics Letters</i> , 2021, 118, .	1.5	7
8	Extended enantiopure <i>ortho</i> -phenylene ethylene (<i>o</i> -OPE)-based helical systems as scaffolds for supramolecular architectures: a study of chiroptical response and its connection to the CISS effect. <i>Organic Chemistry Frontiers</i> , 2021, 8, 5071-5086.	2.3	16
9	Spin Fano Resonances in Chiral Molecules: An Alternative Mechanism for the CISS Effect and Experimental Implications. <i>Nano Letters</i> , 2021, 21, 10423-10430.	4.5	5
10	Field-Mediated Chirality Information Transfer in Molecule–Nanoparticle Hybrids. <i>Journal of Physical Chemistry C</i> , 2020, 124, 1560-1565.	1.5	15
11	Energy localization and excess fluctuations from long-range interactions in equilibrium molecular dynamics. <i>Physica A: Statistical Mechanics and Its Applications</i> , 2020, 540, 123228.	1.2	4
12	Coherence preservation and electron–phonon interaction in electron transfer in DNA. <i>Journal of Chemical Physics</i> , 2020, 153, 165102.	1.2	8
13	Influence of Electronic Structure Modeling and Junction Structure on First-Principles Chiral Induced Spin Selectivity. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 7357-7371.	2.3	31
14	An Ideal Spin Filter: Long-Range, High-Spin Selectivity in Chiral Helicoidal 3-Dimensional Metal Organic Frameworks. <i>Nano Letters</i> , 2020, 20, 8476-8482.	4.5	47
15	Role of Exchange Interactions in the Magnetic Response and Intermolecular Recognition of Chiral Molecules. <i>Nano Letters</i> , 2020, 20, 7077-7086.	4.5	35
16	Enantiospecific Response in Cross-Polarization Solid-State Nuclear Magnetic Resonance of Optically Active Metal Organic Frameworks. <i>Journal of the American Chemical Society</i> , 2020, 142, 17989-17996.	6.6	10
17	Spin-orbit interaction and spin selectivity for tunneling electron transfer in DNA. <i>Physical Review B</i> , 2020, 101, .	1.1	18
18	Carrier Transport Engineering in Carbon Nanotubes by Chirality-Induced Spin Polarization. <i>ACS Nano</i> , 2020, 14, 3389-3396.	7.3	21

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19	Insight into the Origin of Chiral-Induced Spin Selectivity from a Symmetry Analysis of Electronic Transmission. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 2914-2929.	2.3	60
20	Electronic Structure and Triplet-Triplet Energy Transfer in Artificial Photosynthetic Antennas. <i>Photochemistry and Photobiology</i> , 2019, 95, 211-219.	1.3	7
21	Chirality-Induced Spin Selectivity in a Coarse-Grained Tight-Binding Model for Helicene. <i>Journal of Physical Chemistry C</i> , 2019, 123, 27230-27241.	1.5	44
22	Chirality Induced Spin Selectivity of Photoexcited Electrons in Carbon-Sulfur [C _n S _n] Helicenes. <i>ChemPhotoChem</i> , 2019, 3, 770-777.	1.5	14
23	Reply to "Comment on "Chirality-Induced Electron Spin Polarization and Enantiospecific Response in Solid-State Cross-Polarization Nuclear Magnetic Resonance". <i>ACS Nano</i> , 2019, 13, 6133-6136.	7.3	2
24	Selective Transmission of Phonons in Molecular Junctions with Nanoscopic Thermal Baths. <i>Journal of Physical Chemistry C</i> , 2019, 123, 9680-9687.	1.5	7
25	Chirality-Induced Electron Spin Polarization and Enantiospecific Response in Solid-State Cross-Polarization Nuclear Magnetic Resonance. <i>ACS Nano</i> , 2018, 12, 11426-11433.	7.3	21
26	Thermal Decoherence and Disorder Effects on Chiral-Induced Spin Selectivity. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 5753-5758.	2.1	28
27	Enhanced Magnetoresistance in Chiral Molecular Junctions. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 5453-5459.	2.1	69
28	Spin-orbit Coupling Modulation in DNA by Mechanical Deformations. <i>Chimia</i> , 2018, 72, 411.	0.3	24
29	Nanosensors for Biomedical Applications: A Tutorial. <i>Nanostructure Science and Technology</i> , 2018, , 145-167.	0.1	0
30	Gate-controlled conductance switching in DNA. <i>Nature Communications</i> , 2017, 8, 14471.	5.8	103
31	Electrochemical Capture and Release of Carbon Dioxide Using a Disulfide-Thiocarbonate Redox Cycle. <i>Journal of the American Chemical Society</i> , 2017, 139, 1033-1036.	6.6	67
32	Measuring the Spin-Polarization Power of a Single Chiral Molecule. <i>Small</i> , 2017, 13, 1602519.	5.2	143
33	Solvent Effects on the Dynamic Polarizability and Raman Response of Molecule-Metal Oxide Hybrid Clusters. <i>ChemPhysChem</i> , 2016, 17, 2590-2595.	1.0	4
34	Single-Molecule Conductance through Hydrogen Bonds: The Role of Resonances. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 2977-2980.	2.1	16
35	Nonlinear Fano interferences in open quantum systems: An exactly solvable model. <i>Physical Review A</i> , 2016, 93, .	1.0	11
36	Effective spin-orbit couplings in an analytical tight-binding model of DNA: Spin filtering and chiral spin transport. <i>Physical Review B</i> , 2016, 93, .	1.1	72

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37	Polarizability as a Molecular Descriptor for Conductance in Organic Molecular Circuits. <i>Journal of Physical Chemistry C</i> , 2016, 120, 26054-26060.	1.5	16
38	Non-exponential Length Dependence of Conductance in Iodide-Terminated Oligothiophene Single-Molecule Tunneling Junctions. <i>Journal of the American Chemical Society</i> , 2016, 138, 679-687.	6.6	59
39	Fano-Liouville Spectral Signatures in Open Quantum Systems. <i>Physical Review Letters</i> , 2015, 115, 113006.	2.9	16
40	Piezoresistivity in single DNA molecules. <i>Nature Communications</i> , 2015, 6, 8032.	5.8	36
41	Spatial modulation of light transmission through a single microcavity by coupling of photosynthetic complex excitations to surface plasmons. <i>Nature Communications</i> , 2015, 6, 7334.	5.8	20
42	Electronic transport across hydrogen bonds in organic electronics. <i>International Journal of Nanotechnology</i> , 2015, 12, 297.	0.1	7
43	A Nickel Phosphine Complex as a Fast and Efficient Hydrogen Production Catalyst. <i>Journal of the American Chemical Society</i> , 2015, 137, 1109-1115.	6.6	137
44	Intermediate tunnelling "hopping regime in DNA charge transport. <i>Nature Chemistry</i> , 2015, 7, 221-226.	6.6	204
45	Building and testing correlations for the estimation of one-electron reduction potentials of a diverse set of organic molecules. <i>Journal of Physical Organic Chemistry</i> , 2015, 28, 320-328.	0.9	24
46	Chirality transfer takes a jump. <i>Nature Chemistry</i> , 2015, 7, 543-544.	6.6	18
47	Continuum model for chiral induced spin selectivity in helical molecules. <i>Journal of Chemical Physics</i> , 2015, 142, 194308.	1.2	90
48	Inelastic electron scattering from a helical potential: transverse polarization and the structure factor in the single scattering approximation. <i>Journal of Physics Condensed Matter</i> , 2014, 26, 015008.	0.7	28
49	A bioinspired redox relay that mimics radical interactions of the Tyr-His pairs of photosystem II. <i>Nature Chemistry</i> , 2014, 6, 423-428.	6.6	133
50	Probing the Nature of Charge Transfer at Nano-Bio Interfaces: Peptides on Metal Oxide Nanoparticles. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 3555-3559.	2.1	11
51	SERS as a Probe of Charge-Transfer Pathways in Hybrid Dye/Molecule-Metal Oxide Complexes. <i>Journal of Physical Chemistry C</i> , 2014, 118, 3774-3782.	1.5	25
52	The amplifying effect of natural convection on power generation of thermogalvanic cells. <i>International Journal of Heat and Mass Transfer</i> , 2014, 78, 423-434.	2.5	70
53	Dopamine Adsorption on TiO ₂ Anatase Surfaces. <i>Journal of Physical Chemistry C</i> , 2014, 118, 20688-20693.	1.5	47
54	Probing Raman Enhancement in a Dopamine-TiO ₂ O ₄ Hybrid Using Stretched Molecular Geometries. <i>Journal of Physical Chemistry A</i> , 2014, 118, 1196-1202.	1.1	8

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55	Catalytic Hydrogen Evolution by Fe(II) Carbonyls Featuring a Dithiolate and a Chelating Phosphine. <i>Inorganic Chemistry</i> , 2014, 53, 8919-8929.	1.9	39
56	Chemically Induced Magnetism in Atomically Precise Gold Clusters. <i>Small</i> , 2014, 10, 907-911.	5.2	52
57	Kinetic Energy Dependence of Spin Filtering of Electrons Transmitted through Organized Layers of DNA. <i>Journal of Physical Chemistry C</i> , 2013, 117, 22307-22313.	1.5	21
58	Simple and accurate correlation of experimental redox potentials and DFT-calculated HOMO/LUMO energies of polycyclic aromatic hydrocarbons. <i>Journal of Molecular Modeling</i> , 2013, 19, 2845-2848.	0.8	104
59	Gated-Controlled Rectification of a Self-Assembled Monolayer-Based Transistor. <i>Journal of Physical Chemistry C</i> , 2013, 117, 8468-8474.	1.5	38
60	CO ₂ Preactivation in Photoinduced Reduction via Surface Functionalization of TiO ₂ Nanoparticles. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 475-479.	2.1	30
61	Electrode Separation and Operating Orientation: Mechanisms for Maximizing Performance of Cu/Cu ²⁺ Aqueous Thermogalvanic Cells. , 2013, , .		0
62	Chemistry at molecular junctions: Rotation and dissociation of O ₂ on the Ag(110) surface induced by a scanning tunneling microscope. <i>Journal of Chemical Physics</i> , 2013, 139, 074702.	1.2	21
63	Liquid Thermoelectrics: Review of Recent And Limited New Data of Thermogalvanic Cell Experiments. <i>Nanoscale and Microscale Thermophysical Engineering</i> , 2013, 17, 304-323.	1.4	137
64	Electronic and vibrational properties of magnetic core-shell nanoparticles. , 2012, , .		0
65	Optimization of Cell Configuration for Maximizing Performance of a Cu/Cu ²⁺ Aqueous Thermogalvanic Cell. , 2012, , .		1
66	Chiral molecular films as electron polarizers and polarization modulators. <i>Europhysics Letters</i> , 2012, 99, 17006.	0.7	112
67	Stability and Quenching of Plasmon Resonance Absorption in Magnetic Gold Nanoparticles. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 2996-3001.	2.1	5
68	Surface-Enhanced Raman Scattering on Semiconducting Oxide Nanoparticles: Oxide Nature, Size, Solvent, and pH Effects. <i>Journal of Physical Chemistry C</i> , 2011, 115, 8994-9004.	1.5	79
69	Quantum confinement effects on the surface enhanced Raman spectra of hybrid systems molecule@TiO ₂ nanoparticles. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 1659-1670.	1.0	29
70	Exploring local currents in molecular junctions. <i>Nature Chemistry</i> , 2010, 2, 223-228.	6.6	375
71	Mechanistic studies into the Raman enhancement of enediol-semiconducting nanoparticle conjugates and their use in biological applications. <i>Proceedings of SPIE</i> , 2010, , .	0.8	1
72	Ghost transmission: How large basis sets can make electron transport calculations worse. <i>Journal of Chemical Physics</i> , 2010, 132, 024103.	1.2	90

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73	Nonlinear Optical Effects Induced by Nanoparticles in Symmetric Molecules. <i>Journal of Physical Chemistry C</i> , 2010, 114, 20870-20876.	1.5	15
74	Photoinduced Kinetics of SERS in Bioinorganic Hybrid Systems. A Case Study: Dopamine@TiO ₂ . <i>Journal of Physical Chemistry B</i> , 2010, 114, 14642-14645.	1.2	33
75	Gold-Coated Cementite Nanoparticles: An Oxidation-Resistant Alternative to $\hat{\pm}$ -Iron. <i>Chemistry of Materials</i> , 2009, 21, 5594-5600.	3.2	10
76	SERS of Semiconducting Nanoparticles (TiO ₂ Hybrid Composites). <i>Journal of the American Chemical Society</i> , 2009, 131, 6040-6041.	6.6	405
77	Chiral electron transport: Scattering through helical potentials. <i>Journal of Chemical Physics</i> , 2009, 131, 014707.	1.2	151
78	Dipole Orientation and Surface Cluster Size Effects on Chemisorption-Induced Magnetism: A DFT Study of the Interaction of Gold@Thiopolyptide. <i>Journal of Physical Chemistry A</i> , 2008, 112, 9771-9783.	1.1	9
79	Cotunneling Model for Current-Induced Events in Molecular Wires. <i>Nano Letters</i> , 2008, 8, 3525-3531.	4.5	10
80	Dynamics of charge transfer: Rate processes formulated with nonequilibrium Green's functions. <i>Journal of Chemical Physics</i> , 2007, 126, 161103.	1.2	25
81	Laser-induced nonlinear response in photoassisted resonant electronic transport. <i>Journal of Chemical Physics</i> , 2007, 127, 154110.	1.2	17
82	Size dependence of ferromagnetism in gold nanoparticles: Mean field results. <i>Physical Review B</i> , 2007, 76, .	1.1	52
83	Non-Adiabatic Effects in Electron Tunneling in Molecular Junctions. <i>AIP Conference Proceedings</i> , 2007, , .	0.3	0
84	Molecular Conductance Junctions. <i>The Electrical Engineering Handbook</i> , 2007, , 12-1-12-27.	0.2	1
85	Chemisorption-Induced Spin Symmetry Breaking in Gold Clusters and the Onset of Paramagnetism in Capped Gold Nanoparticles. <i>Journal of Physical Chemistry B</i> , 2006, 110, 687-691.	1.2	45
86	Semiconductor/molecule transport junctions: An analytic form for the self-energies. <i>Chemical Physics</i> , 2006, 326, 197-203.	0.9	17
87	A computational study of the stability ratios of spherical colloidal particles. <i>Computational and Theoretical Chemistry</i> , 2006, 769, 165-170.	1.5	8
88	A simple model for laser-electrode interaction and its role in photo-assisted electron transport processes in molecular interfaces. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2005, 38, 3779-3794.	0.6	14
89	Current and noise in a model of an alternating current scanning tunneling microscope molecule-metal junction. <i>Journal of Chemical Physics</i> , 2005, 122, 144703.	1.2	11
90	Laser-assisted conductance of molecular wires: Two-photon contributions. <i>International Journal of Quantum Chemistry</i> , 2004, 99, 460-466.	1.0	10

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91	A Quasimolecular Approach to the Conductance of Molecule~Metal Junctions:~ Theory and Application to Voltage-Induced Conductance Switching. <i>Journal of Physical Chemistry B</i> , 2004, 108, 18414-18420.	1.2	27
92	A Simple Theoretical Model to Study the Voltage Dependence of the Electronic Structure of Phenyl Ethylene Oligomers. <i>Annals of the New York Academy of Sciences</i> , 2003, 1006, 68-81.	1.8	8
93	Molecular Wire Junctions:~ Tuning the Conductance. <i>Journal of Physical Chemistry B</i> , 2003, 107, 91-95.	1.2	55
94	SHG of Ultrathin Films of Metal Porphyrins on BK7 Glass in Total Internal Reflection Geometry:~ Theory and Experiments. <i>Journal of Physical Chemistry B</i> , 2003, 107, 9332-9338.	1.2	3
95	Laser-assisted conductance of molecular wires. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2002, 35, 4981-4988.	0.6	33
96	A Spin Polarization Transfer Approach to Intermolecular Interactions between Hydrocarbon Aromatic Compounds and Free Radicals. <i>Journal of Physical Chemistry A</i> , 2002, 106, 10374-10379.	1.1	1
97	Molecular Rectification in a Metal~Insulator~Metal Junction Based on Self-Assembled Monolayers. <i>Journal of the American Chemical Society</i> , 2002, 124, 11730-11736.	6.6	232
98	Correlating Electron Transport and Molecular Structure in Organic Thin Films. <i>Angewandte Chemie - International Edition</i> , 2002, 41, 382-382.	7.2	1
99	Molecular rectification: why is it so rare?. <i>Chemical Physics</i> , 2002, 281, 147-150.	0.9	128
100	Partitioning technique and transport across molecular interfaces: Many-body effects. <i>International Journal of Quantum Chemistry</i> , 2002, 90, 14-19.	1.0	7
101	Modeling the Electrostatic Potential Spatial Profile of Molecular Junctions. <i>Annals of the New York Academy of Sciences</i> , 2002, 960, 163-176.	1.8	9
102	Correlating Electron Transport and Molecular Structure in Organic Thin Films. <i>Angewandte Chemie - International Edition</i> , 2001, 40, 2316-2320.	7.2	141
103	Nonlinear optical evidences of aggregation in asphaltene~toluene solutions. <i>Fuel</i> , 2001, 80, 1239-1243.	3.4	15
104	Current~voltage characteristics of tunneling molecular junctions for off-resonance injection. <i>Chemical Physics</i> , 2001, 264, 365-370.	0.9	59
105	Correlating Electron Transport and Molecular Structure in Organic Thin Films This work was supported by the Office of Naval Research, the Defense Advanced Research Project Agency, and the National Science Foundation ECS-97294053. R.E.H. thanks the National Institutes of Health for a postdoctoral fellowship, and R.H. thanks the Deutsche Forschungsgemeinschaft and the BASF fellowship program for financial support. We thank Andreas Terfort for the synthesis of aromatic thiol. <i>Collaboration between Caracas and Angewandte Chemie - International Edition</i> , 2001, 40, 2316-2320.	7.2	2
106	Caging of Molecules by Asphaltenes. A Model for Free Radical Preservation in Crude Oils. <i>Energy & Fuels</i> , 2000, 14, 632-639.	2.5	52
107	Molecular wire conductance: Electrostatic potential spatial profile. <i>Journal of Chemical Physics</i> , 2000, 112, 6834-6839.	1.2	198
108	The injecting energy at molecule/metal interfaces: Implications for conductance of molecular junctions from an ab initio molecular description. <i>Journal of Chemical Physics</i> , 1999, 111, 6997-7002.	1.2	261

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109	A Semiempirical Quantum Chemical Study of Some Local Aspects of Ionic Conduction in Poly(ethylene) Tj ETQq1	1.0	78
110	Molecular Wires: Charge Transport, Mechanisms, and Control. Annals of the New York Academy of Sciences, 1998, 852, 22-37.	1.8	79
111	Applications of photothermal displacement spectroscopy to the study of asphaltenes adsorption. Optics Communications, 1998, 145, 69-75.	1.0	21
112	A Conformational Study of the Influence of Vibrations on Conduction in Molecular Wires. Journal of Physical Chemistry B, 1998, 102, 941-947.	1.2	51
113	Non-Born-Oppenheimer corrections in an exactly solvable model of the hydrogen ion molecule. Journal of Physics B: Atomic, Molecular and Optical Physics, 1998, 31, 4537-4544.	0.6	10
114	Molecular Wire Interconnects: Chemical Structural Control, Resonant Tunneling and Length Dependence. VLSI Design, 1998, 8, 65-74.	0.5	1
115	Electron Transfer Rates in Bridged Molecular Systems: A Phenomenological Approach to Relaxation. Journal of Physical Chemistry A, 1997, 101, 6158-6164.	1.1	182
116	Molecular Wires: Resonances, Staircases, Rectification, Bonding and Speculation. , 1997, , 203-217.		0
117	Molecular Wires: Extended Coupling and Disorder Effects. The Journal of Physical Chemistry, 1996, 100, 8349-8355.	2.9	103
118	Current-voltage characteristics of molecular wires: Eigenvalue staircase, Coulomb blockade, and rectification. Journal of Chemical Physics, 1996, 104, 7296-7305.	1.2	300
119	Absorptive and dispersive processes in a two-level molecule with intramolecular coupling and non-zero permanent dipole moment. Journal of Physics B: Atomic, Molecular and Optical Physics, 1994, 27, 4945-4972.	0.6	14
120	Molecular electronics: Disordered molecular wires. Journal of Chemical Physics, 1994, 101, 5172-5178.	1.2	74
121	The effect of intramolecular coupling on the optical susceptibilities of a two-level molecule. Chemical Physics Letters, 1994, 217, 333-341.	1.2	17
122	Resonances and interference effects on the effective electronic coupling in electron transfer. Journal of Photochemistry and Photobiology A: Chemistry, 1994, 82, 81-86.	2.0	19
123	Electron conduction in molecular wires. II. Application to scanning tunneling microscopy. Journal of Chemical Physics, 1994, 101, 6856-6864.	1.2	244
124	Electron conduction in molecular wires. I. A scattering formalism. Journal of Chemical Physics, 1994, 101, 6849-6855.	1.2	479
125	Refractive index in a dilute solution of molecules with intramolecular coupling up to third order in the external field. Molecular Physics, 1994, 82, 227-234.	0.8	10
126	Density Functional Theory in the Context of Local-Scaling Transformations and Its Prospects for Applications in Catalysis. , 1992, , 105-135.		0

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127	Formulation of N - and v -representable density functional theory. IV. Non-Born-Oppenheimer approach. International Journal of Quantum Chemistry, 1991, 40, 589-604.	1.0	24
128	Kohn-Sham theory and the representability problem. Computational and Theoretical Chemistry, 1990, 210, 9-28.	1.5	1
129	Dynamic coordinate separation and state-dependent potentials. An analysis of localization in helium. Chemical Physics, 1987, 112, 159-172.	0.9	8
130	Adiabatic Separation, Broken Symmetries and Geometry Optimization. , 1987, , 597-611.		6
131	Adiabatic coordinate separation and large N -dimensional limit in two-electron ions. International Journal of Quantum Chemistry, 1986, 29, 897-908.	1.0	19
132	Fermion-propagator calculations of excitations in polyenes with the use of a Heisenberg (XYZ) Hamiltonian. II. Applications to large systems. Physical Review B, 1985, 32, 4186-4191.	1.1	5
133	Fermion-propagator calculations of excitations in polyenes with the use of a Heisenberg (XYZ) Hamiltonian. I. Formalism and parametrization. Physical Review B, 1985, 32, 4178-4185.	1.1	10
134	Electron correlation in doubly excited states of helium and extensions to beryllium and magnesium. Chemical Physics, 1984, 87, 473-484.	0.9	6
135	Virial fragments and the Hohenberg-Kohn functional. International Journal of Quantum Chemistry, 1982, 21, 927-935.	1.0	2