Jeffrey A Nichols

List of Publications by Year
in descending order

22	2,762	430874 18	677142 22
papers	citations	h-index	g-index

22	22	22	3213
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Ionization Potential, Electron Affinity, Electronegativity, Hardness, and Electron Excitation Energy:â€‰Molecular Properties from Density Functional Theory Orbital Energies. Journal of Physical Chemistry A, 2003, 107, 4184-4195.	2.5	1,134
2	High performance computational chemistry: An overview of NWChem a distributed parallel application. Computer Physics Communications, 2000, 128, 260-283.	7.5	698
3	Comparison of perturbative and multiconfigurational electron propagator methods. International Journal of Quantum Chemistry, 1996, 60, 29-36.	2.0	200
4	Complexation of the Carbonate, Nitrate, and Acetate Anions with the Uranyl Dication:Â Density Functional Studies with Relativistic Effective Core Potentialsâ€. Journal of Physical Chemistry A, 2005, 109, 11568-11577.	2.5	100
5	The optimized effective potential and the self-interaction correction in density functional theory: Application to molecules. Journal of Chemical Physics, 2000, 112, 7880-7890.	3.0	96
6	Multiconfigurational electron propagator (MCEP) ionization potentials for general open shell systems. Journal of Chemical Physics, 1984, 80, 293-314.	3.0	87
7	Orbital energy analysis with respect to LDA and self-interaction corrected exchange-only potentials. Journal of Chemical Physics, 2001, 114, 639.	3.0	63
8	Photoionization cross sections involving an explicitly correlated initial state: Combination of multiconfigurational linear response and the stieltjesâ€”tchebycheff moment theory. Chemical Physics, 1986, 110, 339-354.	1.9	42
9	The role of the local-multiplicative Kohnâ€“Sham potential on the description of occupied and unoccupied orbitals. Journal of Chemical Physics, 2000, 113, 6029-6034.	3.0	41
10	Combined Quantum Chemistry and Photoelectron Spectroscopy Study of the Electronic Structure and Reduction Potentials of Rubredoxin Redox Site Analogues. Journal of Physical Chemistry A, 2003, 107, 2898-2907.	2.5	39
11	Multiconfigurational spin tensor electron propagator electron affinities for F, BO, CN, OH, and NH2. Journal of Chemical Physics, 1992, 97, 8441-8448.	3.0	32
12	Complete basis set limit ionization potentials of O3 and NO2 using the multiconfigurational spin tensor electron propagator method (MCSTEP). Chemical Physics, 1998, 238, 1-9.	1.9	32
13	The ionization potentials of F2:â€‰A comparison of multiconfigurational electron propagator (MCEP) with other large scale methods using the same basis set. Journal of Chemical Physics, 1986, 84, 284-299.	3.0	30
14	Ionization potentials of CH2: A comparison of the multiconfigurational spin tensor electron propagator method with benchmark full configuration interaction and large scale multireference configuration interaction calculations. Journal of Chemical Physics, 1994, 100, 2947-2952.	3.0	24
15	The potential energy curves of theXâ€‰2Îg,aâ€‰4Îu,Aâ€‰2Îu,bâ€‰4Î£â^'g,Bâ€‰2Î£â^'g,2Îu, andcâ€‰4Î£â^'ustates of O+2obtained multiconfigurational spin tensor electron propagator method. Journal of Chemical Physics, 1994, 100, 6514-6519.	3.0	24
16	The determination of electron affinities of the open shell systems C and CH2using the multiconfigurational spin tensor electron propagator method. Journal of Chemical Physics, 1993, 98, 8790-8800.	3.0	22
17	The Hartree product and the description of local and global quantities in atomic systems: A study within Kohnâ€“Sham theory. Journal of Chemical Physics, 2000, 112, 1150-1157.	3.0	22
18	The multiconfigurational spin tensor electron propagator method (MCSTEP): Comparison with extended Koopmans' theorem results. Theoretica Chimica Acta, 1995, 90, 273-290.	0.8	19

#	Article	IF	Citations
19	Methylene excitation energies, transition probabilities, and frequency dependent polarizabilities. Chemical Physics Letters, 1981, 84, 77-85.	2.6	15
20	Lowâ€lying ionization potentials of O3and NO2using the multiconfigurational spin tensor electron propagator method. Journal of Chemical Physics, 1996, 105, 9927-9932.	3.0	15
21	Optimization of Spin-Unrestricted Density Functional Theory for Redox Properties of Rubredoxin Redox Site Analogues. Journal of Chemical Theory and Computation, 2009, 5, 1361-1368.	5.3	15
22	Relationship between singletâ€“triplet excitation energies and the Kohnâ€“Sham orbitals obtained with potentials that exhibit a wrong asymptotic behavior. Chemical Physics Letters, 2006, 419, 207-212.	2.6	12