Walter C Ermler

List of Publications by Year
in descending order

23 papers	918 citations	1040056 9 h-index	794594 19 g-index
25 all docs	25 docs citations	25 times ranked	464 citing authors

#	Article	IF	Citations
1	Spinâ€“orbit configuration interaction study of spectral properties of PbO. Journal of Physics Condensed Matter, 2022, 34, 344003.	1.8	0
2	jj-Coupling-based atomic self-consistent-field calculations with relativistic effective core potentials and two-component spinors. Computer Physics Communications, 2018, 229, 182-198.	7.5	0
3	Massively parallel spinâ€“orbit configuration interaction. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	9
4	Generally contracted valenceâ€“core/valence basis sets for use with relativistic effective core potentials and spinâ€“orbit coupling operators. Computational and Theoretical Chemistry, 2012, 1002, 24-30.	2.5	4
5	CI potential energy curves for three states of RuO2+. Chemical Physics Letters, 2011, 516, 131-136.	2.6	4
6	Ab initio study of AmCl+: fâ€“f spectroscopy and chemical binding. Journal of Chemical Physics, 2004, 121, 5661-5675.	3.0	4
7	An ab initio study of the fâ€“f spectroscopy of americium +3. Journal of Chemical Physics, 2002, 116, 5494-5502.	3.0	5
8	Nodeless Valence (Pseudo)spinors. Journal of Chemical Information and Computer Sciences, 2001, 41, 77-82.	2.8	7
9	Ab initio determination of americium ionization potentials. Journal of Chemical Physics, 2000, 112, 2292-2300.	3.0	5
10	Ab initiorelativistic effective potentials with spin-orbit operators. VII. Am through element 118. Journal of Chemical Physics, 1997, 106, 5133-5142.	3.0	107
11	Ab initio relativistic effective potentials with spinâ€“orbit operators. V. Ce through Lu. Journal of Chemical Physics, 1994, 100, 8145-8155.	3.0	106
12	Ab initio effective core potentials including relativistic effects.: II. Potential energy curves for Xe2, ${m Xe}^+_2$, and Xe*2. World Scientific Series in 20th Century Chemistry, 1993, , 128-135.	0.0	0
13	Ab initio effective core potentials including relativistic effects.: III. Ground state Au2 calculations. World Scientific Series in 20th Century Chemistry, 1993, , 136-140.	0.0	0
14	Ab initio effective core potentials including relativistic effects.: IV. Potential energy curves for the ground and several excited states of Au₂. World Scientific Series in 20th Century Chemistry, 1993, , 141-146.	0.0	0
15	Ab initio effective core potentials including relativistic effects.: V. SCF calculations with Ï‰â€“Ï‰ coupling including results for Au₂⁺, TlH, PbS, and PbSe. World Scientific Series in 20th Century Chemistry, 1993, , 159-165.	0.0	2
16	AB INITIO EFFECTIVE CORE POTENTIALS INCLUDING RELATIVISTIC EFFECTS.: A PROCEDURE FOR THE INCLUSION OF SPINâ€“ORBIT COUPLING IN MOLECULAR WAVEFUNCTIONS. World Scientific Series in 20th Century Chemistry, 1993, , 176-180.	0.0	1
17	Ab initio vibrational transition dipole moments and intensities of formaldehyde. Journal of Computational Chemistry, 1988, 9, 95-106.	3.3	11
18	Electronic states and geometries of small Be clusters. Journal of Chemical Physics, 1987, 86, 6283-6294.	3.0	39

#	Article	IF	Citations
19	Polyatomic, anharmonic, vibrational-rotational analysis. Application to accurateab initio results for formaldehyde. Journal of Computational Chemistry, 1985, 6, 13-27.	3.3	103
20	Ab initio calculations of potential energy curves of Hg2 and TlHg. Journal of Chemical Physics, 1984, 81, 1872-1881.	3.0	40
21	AB initio effective core potentials including relativistic effects. A procedure for the inclusion of spin-orbit coupling in molecular wavefunctions. Chemical Physics Letters, 1981, 81, 70-74.	2.6	145
22	Ab initio effective core potentials including relativistic effects. V. SCF calculations with ï‰â€“ï‰ coupling including results for Au2+, TlH, PbS, and PbSe. Journal of Chemical Physics, 1980, 73, 360-366.	3.0	72
23	Ab initio effective core potentials including relativistic effects. I. Formalism and applications to the Xe and Au atoms. Journal of Chemical Physics, 1977, 67, 5861-5876.	3.0	245