Hermann Stoll

List of Publications by Citations

95 papers	29,794 citations	52 h-index	97 g-index
97 ext. papers	32,269 ext. citations	4 avg, IF	6.69 L-index

#	Paper	IF	Citations
95	Energy-adjustedab initio pseudopotentials for the second and third row transition elements. *Theoretica Chimica Acta*, **1990**, 77, 123-141		6599
94	Energy-adjusted ab initio pseudopotentials for the first row transition elements. *Journal of Chemical Physics*, **1987**, 86, 866-872	3.9	2632
93	Ab initio energy-adjusted pseudopotentials for elements of groups 13–17. *Molecular Physics*, **1993**, 80, 1431-1441	1.7	2334
92	Systematically convergent basis sets with relativistic pseudopotentials. II. Small-core pseudopotentials and correlation consistent basis sets for the post-d group 16–18 elements. *Journal of Chemical Physics*, **2003**, 119, 11113-11123	3.9	1590
91	Energy-adjusted pseudopotentials for the actinides. Parameter sets and test calculations for thorium and thorium monoxide. *Journal of Chemical Physics*, **1994**, 100, 7535-7542	3.9	1289
90	Energy-adjusted pseudopotentials for the rare earth elements. *Theoretica Chimica Acta*, **1989**, 75, 173-194		971
89	Small-core multiconfiguration-Dirac–Hartree–Fock-adjusted pseudopotentials for post-d main group elements: Application to PbH and PbO. *Journal of Chemical Physics*, **2000**, 113, 2563-2569	3.9	869
88	Energy-adjusted ab initio pseudopotentials for the rare earth elements. *Journal of Chemical Physics*, **1989**, 90, 1730-1734	3.9	817
87	A proper account of core-polarization with pseudopotentials: single valence-electron alkali compounds. *Chemical Physics Letters*, **1982**, 89, 418-422	2.5	768
86	Energy-consistent pseudopotentials for group 11 and 12 atoms: adjustment to multi-configuration Dirac–Hartree–Fock data. *Chemical Physics*, **2005**, 311, 227-244	2.3	763
85	Energy-consistent relativistic pseudopotentials and correlation consistent basis sets for the 4d elements Y-Pd. *Journal of Chemical Physics*, **2007**, 126, 124101	3.9	714
84	Magnetic vortex core reversal by excitation with short bursts of an alternating field. *Nature*, **2006**, 444, 461-4	50.4	675
83	A combination of quasirelativistic pseudopotential and ligand field calculations for lanthanoid compounds. *Theoretica Chimica Acta*, **1993**, 85, 441-450		612
82	Relativistic and correlation effects for element 105 (hahnium, Ha): a comparative study of M and MO (M = Nb, Ta, Ha) using energy-adjusted ab initio pseudopotentials. *The Journal of Physical Chemistry*, **1993**, 97, 5852-5859		608
81	On the spectroscopic and thermochemical properties of ClO, BrO, IO, and their anions. *Journal of Physical Chemistry A*, **2006**, 110, 13877-83	2.8	606
80	Valence basis sets for relativistic energy-consistent small-core actinide pseudopotentials. *Journal of Chemical Physics*, **2003**, 118, 487-496	3.9	518
79	Pseudopotential approaches to Ca, Sr, and Ba hydrides. Why are some alkaline earth MX2 compounds bent?. *Journal of Chemical Physics*, **1991**, 94, 1360-1366	3.9	502

78	Energy-consistent pseudopotentials and correlation consistent basis sets for the 5d elements Hf-Pt. *Journal of Chemical Physics*, **2009**, 130, 164108	3.9	483
77	Ab initio pseudopotentials for Hg through Rn. *Molecular Physics*, **1991**, 74, 1245-1263	1.7	469
76	Ab initio energy-adjusted pseudopotentials for the noble gases Ne through Xe: Calculation of atomic dipole and quadrupole polarizabilities. *Journal of Chemical Physics*, **1995**, 102, 8942-8952	3.9	434
75	The accuracy of the pseudopotential approximation. II. A comparison of various core sizes for indium pseudopotentials in calculations for spectroscopic constants of InH, InF, and InCl. *Journal of Chemical Physics*, **1996**, 105, 1052-1059	3.9	434
74	Pseudopotentials for main group elements (IIIa through VIIa). *Molecular Physics*, **1988**, 65, 1321-1328	1.7	368
73	Correlation energy of diamond. *Physical Review B*, **1992**, 46, 6700-6704	3.3	343
72	Accuracy of energy-adjusted quasirelativistic ab initio pseudopotentials. *Molecular Physics*, **1993**, 78, 1211-1224	1.7	342
71	The accuracy of the pseudopotential approximation: non-frozen-core effects for spectroscopic constants of alkali fluorides XF (X = K, Rb, Cs). *Chemical Physics Letters*, **1996**, 255, 274-280	2.5	255
70	The correlation energy of crystalline silicon. *Chemical Physics Letters*, **1992**, 191, 548-552	2.5	241
69	Pseudopotential calculations on Rb+2, Cs+2, RbH+, CsH+ and the mixed alkali dimer ions. *Chemical Physics Letters*, **1982**, 93, 555-559	2.5	212
68	Pseudopotential calculations for alkaline-earth atoms. *Journal of Physics B: Atomic and Molecular Physics*, **1985**, 18, 1287-1296		196
67	On the correlation energy of graphite. *Journal of Chemical Physics*, **1992**, 97, 8449-8454	3.9	188
66	Relativistic energy-consistent pseudopotentials--recent developments. *Journal of Computational Chemistry*, **2002**, 23, 767-78	3.5	184
65	Magnetic vortex core reversal by excitation of spin waves. *Nature Communications*, **2011**, 2, 279	17.4	178
64	Relativistic small-core energy-consistent pseudopotentials for the alkaline-earth elements from Ca to Ra. *Journal of Chemical Physics*, **2006**, 124, 034107	3.9	160
63	On the reliability of semi-empirical pseudopotentials: simulation of Hartree-Fock and Dirac-Fock results. *Journal of Physics B: Atomic and Molecular Physics*, **1983**, 16, L323-L328		147
62	Ground state calculations of di-π-cyclooctatetraene cerium. *Journal of Chemical Physics*, **1991**, 94, 3011-3017	3.9	143
61	A small-core multiconfiguration Dirac–Hartree–Fock-adjusted pseudopotential for Tl application to TlX (X = F, Cl, Br, I). *Theoretical Chemistry Accounts*, **2000**, 104, 22-28	1.9	122

60	Ab initio calculation of ground-state properties of rare-gas crystals. *Physical Review B*, **1999**, 60, 7905-7910	3.3	114
59	On the accuracy of correlation-energy expansions in terms of local increments. *Journal of Chemical Physics*, **2005**, 123, 144108	3.9	110
58	Ab initio coupled-cluster calculations for the fcc and hcp structures of rare-gas solids. *Physical Review B*, **2000**, 62, 5482-5488	3.3	105
57	Cu and Ag as one-valence-electron atoms: CI results and quadrupole corrections for Cu2, Ag2, CuH, and AgH. *Journal of Chemical Physics*, **1984**, 81, 2732-2736	3.9	97
56	Vortex core switching by coherent excitation with single in-plane magnetic field pulses. *Physical Review Letters*, **2009**, 102, 077201	7.4	83
55	Correlation effects in ionic crystals: The cohesive energy of MgO. *Physical Review B*, **1995**, 52, 4842-4848	3.3	81
54	The accuracy of the pseudopotential approximation. III. A comparison between pseudopotential and all-electron methods for Au and AuH. *Journal of Chemical Physics*, **2000**, 113, 7110-7118	3.9	76
53	Wave-function-based correlated ab initio calculations on crystalline solids. *Physical Review B*, **1999**, 60, 5211-5216	3.3	71
52	Spin-orbit interaction in heavy group 13 atoms and TlAr. *Chemical Physics*, **1997**, 217, 19-27	2.3	70
51	The accuracy of the pseudopotential approximation. I. An analysis of the spectroscopic constants for the electronic ground states of InCl and InCl3 using various three valence electron pseudopotentials for indium. *Journal of Chemical Physics*, **1995**, 102, 2050-2062	3.9	70
50	Ab initio pseudopotentials for Hg to Rn. *Molecular Physics*, **1991**, 74, 1265-1285	1.7	68
49	Quantum chemical approach to cohesive properties of NiO. *Physical Review B*, **1997**, 55, 10282-10288	3.3	64
48	Convergence of the ab initio many-body expansion for the cohesive energy of solid mercury. *Physical Review B*, **2004**, 70,	3.3	64
47	Closed-shell interaction in silver and gold chlorides. *Journal of Chemical Physics*, **1998**, 109, 2339-2345	3.9	60
46	Electron correlations for ground-state properties of group-IV semiconductors. *Physical Review B*, **1995**, 51, 10572-10578	3.3	56
45	Correlation effects in MgO and CaO: Cohesive energies and lattice constants. *Physical Review B*, **1996**, 54, 13529-13535	3.3	55
44	Lattice structure of mercury: Influence of electronic correlation. *Physical Review B*, **2006**, 74,	3.3	54
43	Electronic structure and spectroscopy of monohalides of metals of group I-B. *Chemical Physics*, **2002**, 280, 71-102	2.3	52

42	Semi-local pseudopotential calculations for the adiabatic potentials of alkali-neon systems. *Chemical Physics*, **1989**, 136, 79-94	2.3	51
41	An incremental correlation approach to excited state energies based on natural transition/localized orbitals. *Journal of Chemical Physics*, **2011**, 134, 034122	3.9	43
40	Imaging spin dynamics on the nanoscale using X-Ray microscopy. *Frontiers in Physics*, **2015**, 3,	3.9	39
39	Cohesive properties of alkali halides. *Physical Review B*, **1997**, 56, 10121-10127	3.3	37
38	Coherent Excitation of Heterosymmetric Spin Waves with Ultrashort Wavelengths. *Physical Review Letters*, **2019**, 122, 117202	7.4	36
37	Ground-state properties of heavy alkali halides. *Physical Review B*, **1998**, 57, 4327-4331	3.3	35
36	Adiabatic potential curves for the Cd2 dimer. *Chemical Physics Letters*, **1994**, 225, 233-239	2.5	33
35	Improved dipole moments by combining short-range gradient-corrected density-functional theory with long-range wave-function methods. *Physical Review A*, **2007**, 76,	2.6	30
34	Combining density functional and incremental post-Hartree-Fock approaches for van der Waals dominated adsorbate-surface interactions: Ag2/graphene. *Journal of Chemical Physics*, **2015**, 143, 102804	3.9	26
33	Adsorption of Benzene to Copper in CuHY Zeolite. *Journal of Physical Chemistry C*, **2009**, 113, 4107-4116	3.8	25
32	On the performance of energy-consistent spin□rbit pseudopotentials: (111)H revisited. *Chemical Physics Letters*, **2001**, 345, 490-496	2.5	23
31	An incremental coupled-cluster approach to metallic lithium. *Chemical Physics Letters*, **2009**, 469, 90-93	2.5	22
30	On the coupling of multi-configuration self-consistent-field and density-functional information. *Chemical Physics Letters*, **2003**, 376, 141-147	2.5	22
29	Unidirectional sub-100-ps magnetic vortex core reversal. *Physical Review B*, **2014**, 90,	3.3	20
28	Approaching the bulk limit with finite cluster calculations using local increments: the case of LiH. *Journal of Chemical Physics*, **2012**, 136, 074106	3.9	19
27	On the importance of core polarization in heavy post-d elements: a pseudopotential calibration study for X2H6 (X = Si, Ge, Sn, Pb). *Molecular Physics*, **1995**, 86, 317-326	1.7	19
26	Direct observation of coherent magnons with suboptical wavelengths in a single-crystalline ferrimagnetic insulator. *Physical Review B*, **2019**, 100,	3.3	19
25	Adsorption of dioxygen to copper in CuHY zeolite. *Physical Chemistry Chemical Physics*, **2009**, 11, 8855-66	3.6	17

24	Dealing with the exponential wall in electronic structure calculations. *Journal of Chemical Physics*, **2017**, 146, 194107	3.9	14
23	Can incremental expansions cope with high-order coupled-cluster contributions?. *Molecular Physics*, **2010**, 108, 243-248	1.7	14
22	Energy-consistent pseudopotentials for the 5d elements--benchmark calculations for oxides, nitrides, and Pt(2). *Journal of Physical Chemistry A*, **2009**, 113, 12478-84	2.8	13
21	On the performance of two-component energy-consistent pseudopotentials in atomic Fock-space coupled cluster calculations. *Journal of Chemical Physics*, **2008**, 128, 024106	3.9	13
20	Calculated spectroscopic properties of HgH2. *Molecular Physics*, **2007**, 105, 1193-1205	1.7	13
19	Nanoscale X-ray imaging of spin dynamics in yttrium iron garnet. *Journal of Applied Physics*, **2019**, 126, 173909	2.5	12
18	Simultaneous adsorption of benzene and dioxygen in CuHY zeolites as a precursor process to the aerobic oxidation of benzene to phenol. *Physical Chemistry Chemical Physics*, **2010**, 12, 6345-51	3.6	11
17	Large-core vs. small-core pseudopotentials: A case study for Au2. *Chemical Physics Letters*, **2006**, 429, 289-293	2.5	10
16	A systematic ab initio study of the equilibrium geometry and vibrational wave numbers of bismuthine. *Journal of Chemical Physics*, **2004**, 120, 10404-13	3.9	9
15	Toward a wave-function-based treatment of metals: extrapolation from finite clusters. *Journal of Physical Chemistry A*, **2009**, 113, 11483-6	2.8	7
14	Transferable Scaling Factors for Vibrational Force Fields of Halogenated Molecules Based on Energy-Consistent Pseudopotentials. *Journal of Physical Chemistry A*, **2002**, 106, 6810-6816	2.8	7
13	Toward a wavefunction-based treatment of strong electron correlation in extended systems by means of incremental methods. *Journal of Chemical Physics*, **2019**, 151, 044104	3.9	6
12	A theoretical study of ZnH2: a case of very strong Darling□Dennison resonance. *Molecular Physics*, **2010**, 108, 487-499	1.7	6
11	Towards an incremental expansion of strong correlation effects in solids. *Annalen Der Physik*, **2010**, 508, 355-362	2.6	6
10	Quantification of Competing Magnetic States and Switching Pathways in Curved Nanowires by Direct Dynamic Imaging. *ACS Nano*, **2020**, 14, 13324-13332	16.7	5
9	Accurate potential energy surface and calculated spectroscopic properties for CdH2 isotopomers. *Journal of Physical Chemistry A*, **2009**, 113, 11772-82	2.8	4
8	Comment on □Atomization energies and enthalpies of formation of the SnBin (n=1□3) gaseous molecules by Knudsen cell mass spectrometry□[J. Chem. Phys. 116, 6957 (2002)]. *Journal of Chemical Physics*, **2003**, 118, 4766-4767	3.9	4
7	Direct Imaging of High-Frequency Multimode Spin Wave Propagation in Cobalt-Iron Waveguides Using X-Ray Microscopy beyond 10 GHz. *Physica Status Solidi - Rapid Research Letters*, **2020**, 14, 2000373	2.5	3

6	Extrapolating wavefunction-based ab initio results from finite clusters to the bulk solid The case of group 1 and 11 metals (Li,Cu). *Chemical Physics Letters*, **2011**, 501, 283-286	2.5	2
5	Filling the Gap between Pseudopotential and All-Electron Schemes: Frozen-Core Calculations with Efficient Use of Density-Fitting. *Journal of Chemical Theory and Computation*, **2014**, 10, 3857-62	6.4	1
4	Magnetic State Control via Field-Angle-Selective Switching in Asymmetric Rings. *Physical Review Applied*, **2020**, 14,	4.3	1
3	Ptychographic imaging and micromagnetic modeling of thermal melting of nanoscale magnetic domains in antidot lattices. *AIP Advances*, **2020**, 10, 125122	1.5	1
2	All-electron-derived pseudopotentials for embedding: the polarisability of the iodine anion in a water cage. *Molecular Physics*, **2016**, 114, 941-946	1.7	
1	On the accuracy of small-core and large-core pseudopotentials **2006**, 973-974		