Pekka Pyykk

List of Publications by Citations

214 papers	22,970 citations	65 h-index	149 g-index
219 ext. papers	24,479 ext. citations	6.5 avg, IF	7.7 L-index

#	Paper	IF	Citations
214	Relativistic effects in structural chemistry. *Chemical Reviews*, **1988**, 88, 563-594	68.1	2438
213	Strong Closed-Shell Interactions in Inorganic Chemistry. *Chemical Reviews*, **1997**, 97, 597-636	68.1	2065
212	Theoretical chemistry of gold. *Angewandte Chemie - International Edition*, **2004**, 43, 4412-56	16.4	1550
211	Molecular single-bond covalent radii for elements 1-118. *Chemistry - A European Journal*, **2009**, 15, 186-97	4.8	1416
210	Molecular double-bond covalent radii for elements Li-E112. *Chemistry - A European Journal*, **2009**, 15, 12770-9	4.8	912
209	Relativity and the periodic system of elements. *Accounts of Chemical Research*, **1979**, 12, 276-281	24.3	885
208	Theoretical chemistry of gold. III. *Chemical Society Reviews*, **2008**, 37, 1967-97	58.5	574
207	Spectroscopic nuclear quadrupole moments. *Molecular Physics*, **2001**, 99, 1617-1629	1.7	477
206	Year-2008 nuclear quadrupole moments. *Molecular Physics*, **2008**, 106, 1965-1974	1.7	400
205	Theory of the d10–d10 Closed-Shell Attraction: 1. Dimers Near Equilibrium. *Chemistry - A European Journal*, **1997**, 3, 1451-1457	4.8	386
204	Theoretical chemistry of gold. II. *Inorganica Chimica Acta*, **2005**, 358, 4113-4130	2.7	373
203	Additive covalent radii for single-, double-, and triple-bonded molecules and tetrahedrally bonded crystals: a summary. *Journal of Physical Chemistry A*, **2015**, 119, 2326-37	2.8	340
202	Molecular tweezers for hydrogen: synthesis, characterization, and reactivity. *Journal of the American Chemical Society*, **2008**, 130, 14117-9	16.4	332
201	Relativistic effects in chemistry: more common than you thought. *Annual Review of Physical Chemistry*, **2012**, 63, 45-64	15.7	330
200	Triple-bond covalent radii. *Chemistry - A European Journal*, **2005**, 11, 3511-20	4.8	327
199	Icosahedral WAu12: a predicted closed-shell species, stabilized by aurophilic attraction and relativity and in accord with the 18-electron rule. *Angewandte Chemie - International Edition*, **2002**, 41, 2174-6	16.4	315
198	Relativistic Quantum Chemistry. *Advances in Quantum Chemistry*, **1978**, 11, 353-409	1.4	307

197	How Do Spin–Orbit-Induced Heavy-Atom Effects on NMR Chemical Shifts Function? Validation of a Simple Analogy to Spin–Spin Coupling by Density Functional Theory (DFT) Calculations on Some Iodo Compounds. *Chemistry - A European Journal*, **1998**, 4, 118-126	4.8	305
196	Theoretische Chemie des Golds. *Angewandte Chemie*, **2004**, 116, 4512-4557	3.6	277
195	Predicted ligand dependence of the Au(I)···Au(I) attraction in (XAuPH3)2. *Chemical Physics Letters*, **1994**, 218, 133-138	2.5	235
194	Fully numerical hartree-fock methods for molecules. *Computer Physics Reports*, **1986**, 4, 313-344		229
193	Cationic Gold(I) Complexes of Xenon and of Ligands Containing the Donor Atoms Oxygen, Nitrogen, Phosphorus, and Sulfur. *Inorganic Chemistry*, **1998**, 37, 624-632	5.1	228
192	Ab initio Calculations on the (ClAuPH3)2 Dimer with Relativistic Pseudopotential: Is the "Aurophilic Attraction" a Correlation Effect?. *Angewandte Chemie International Edition in English*, **1991**, 30, 604-605		211
191	Theory of d10–d10 Closed-Shell Attraction. III. Rings. *Inorganic Chemistry*, **1998**, 37, 3018-3025	5.1	190
190	The Nuclear Quadrupole Moments of the 20 First Elements: High-Precision Calculations on Atoms and Small Molecules. *Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences*, **1992**, 47, 189-196	1.4	183
189	Relativity, gold, closed-shell interactions, and CsAu.NH3. *Angewandte Chemie - International Edition*, **2002**, 41, 3573-8, 3512	16.4	169
188	Ab initio studies of the dimers (HgH2)2 and (HgMe2)2. Metallophilic attraction and the van der Waals radii of mercury. *Physical Chemistry Chemical Physics*, **2000**, 2, 2489-2493	3.6	163
187	Theory of the d10–d10 Closed-Shell Attraction: 2. Long-Distance Behaviour and Nonadditive Effects in Dimers and Trimers of Type [(x-Au-L)n] (n = 2, 3; X = Cl, I, H; L = PH3, PMe3, -N?CH). *Chemistry - A European Journal*, **1997**, 3, 1458-1465	4.8	162
186	The physics behind chemistry and the periodic table. *Chemical Reviews*, **2012**, 112, 371-84	68.1	149
185	A transparent interpretation of the relativistic contribution to the N.M.R. "heavy atom chemical shift". *Molecular Physics*, **1987**, 61, 195-205	1.7	147
184	Understanding the eighteen-electron rule. *Journal of Organometallic Chemistry*, **2006**, 691, 4336-4340	2.3	139
183	Luminescent Characterization of Solution Oligomerization Process Mediated Gold–Gold Interactions. DFT Calculations on [Au2Ag2R4L2]n Moieties. *Journal of the American Chemical Society*, **2000**, 122, 7287-7293	16.4	126
182	Matrix Infrared Spectroscopic and ab Initio Studies of ZnH2, CdH2, and Related Metal Hydride Species. *The Journal of Physical Chemistry*, **1995**, 99, 7925-7934		109
181	Relativistic pseudo-potential analysis of the weak Au(I)···Au(I) attraction. *Chemical Physics Letters*, **1992**, 197, 586-590	2.5	107
180	Two-dimensional, fully numerical molecular calculations. *Molecular Physics*, **1985**, 56, 1411-1418	1.7	106

179	A suggested periodic table up to Z = 172, based on Dirac-Fock calculations on atoms and ions. *Physical Chemistry Chemical Physics*, **2011**, 13, 161-8	3.6	105
178	Calculated energy levels of thallium and eka-thallium (element 113). *Physical Review A*, **1996**, 53, 3926-3933	2.8	100
177	Relativistic, nearly basis-set-limit nuclear magnetic shielding constants of the rare gases He–Rn: A way to absolute nuclear magnetic resonance shielding scales. *Journal of Chemical Physics*, **2003**, 118, 2973-2976	3.9	98
176	Aurophilicity: the effect of the neutral ligand L on [{ClAuL}(2)] systems. *Chemistry - A European Journal*, **2011**, 17, 368-77	4.8	97
175	A predicted organometallic series following a 32-electron principle: An@C28 (An = Th, Pa+, U2+, Pu4+). *Journal of the American Chemical Society*, **2009**, 131, 238-43	16.4	96
174	Icosahedral Au(72): a predicted chiral and spherically aromatic golden fullerene. *Chemical Communications*, **2008**, 465-7	5.8	95
173	Properties of WAu12. *Physical Chemistry Chemical Physics*, **2004**, 6, 11-22	3.6	93
172	Element 118: The First Rare Gas with an Electron Affinity. *Physical Review Letters*, **1996**, 77, 5350-5352	7.4	93
171	Ab Initio Interpretation of the Closed-Shell Intermolecular E.cntdot..cntdot..cntdot.E Attraction in Dipnicogen (H2E-EH2)2 and Dichalcogen (HE-EH)2 Hydride Model Dimers. *Inorganic Chemistry*, **1995**, 34, 4134-4138	5.1	91
170	Experimental and theoretical treatment of hydrogen splitting and storage in boron–nitrogen systems. *Journal of Organometallic Chemistry*, **2009**, 694, 2654-2660	2.3	86
169	Trends in inversion barriers. I. Group-15 hydrides. *Journal of Chemical Physics*, **1992**, 96, 6807-6819	3.9	84
168	Ab initio study of bonding trends for f0 actinide oxyfluoride species. *Theoretical Chemistry Accounts*, **2001**, 106, 393-403	1.9	83
167	How many hydrogen atoms can be bound to a metal? Predicted MH12 species. *Journal of the American Chemical Society*, **2004**, 126, 15014-5	16.4	82
166	Relativity and the lead-acid battery. *Physical Review Letters*, **2011**, 106, 018301	7.4	80
165	Ab-initio-Rechnungen am Dimer (ClAuPH3)2 mit relativistischem Pseudopotential: Ist die Aurophile Attraktion ein Korrelationseffekt?. *Angewandte Chemie*, **1991**, 103, 622-623	3.6	80
164	Dirac–Fock one-centre calculations. Part 7.—Divalent systems MH+ and MH2(M = Be, Mg, Ca, Sr, Ba, Ra, Zn, Cd, Hg, Yb and No). *Journal of the Chemical Society, Faraday Transactions 2*, **1979**, 75, 1256-1276		80
163	Towards a 32-electron principle: Pu@Pb12 and related systems. *Angewandte Chemie - International Edition*, **2007**, 46, 1427-30	16.4	78
162	Nuclear quadrupole moment of lithium from combined fully numerical and discrete basis-set calculations on LiH. *Chemical Physics Letters*, **1984**, 112, 1-9	2.5	78

161	Estimation of Lamb-shift effects for molecules: Application to the rotation-vibration spectra of water. *Physical Review A*, **2001**, 63,	2.6	76
160	Why are hexavalent uranium cyanides rare while U≡E and U≡O bonds are common and short?. *Theoretical Chemistry Accounts*, **2003**, 109, 332-340	1.9	75
159	[-N5-]2[Metal(2+)-N73-]: A New Class of Compounds. *Journal of Physical Chemistry A*, **2002**, 106, 4690-4694	2.8	75
158	Structure of tetrakis(phosphine)nitrido- or -phosphinidyne or arsinidyneultragold(1+): Td or C4v?. *Inorganic Chemistry*, **1993**, 32, 2630-2634	5.1	73
157	A very short uranium-uranium bond: the predicted metastable U(2)2+. *Physical Chemistry Chemical Physics*, **2005**, 7, 2415-7	3.6	71
156	Aurophilic attraction in binuclear complexes with Au(I) and Au(III). A theoretical study. *Physical Chemistry Chemical Physics*, **2004**, 6, 900-905	3.6	71
155	Theory of the d10−d10Closed-Shell Attraction. 4. X(AuL)nm+Centered Systems. *Organometallics*, **1998**, 17, 4842-4852	3.8	70
154	Ab initio studies of bonding trends. *Computational and Theoretical Chemistry*, **1991**, 234, 279-290		69
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151	Electric quadrupole moment of the 27Al nucleus: Converging results from the AlF and AlCl molecules and the Al atom. *Chemical Physics Letters*, **1999**, 304, 414-422	2.5	67
150	Year-2017 nuclear quadrupole moments. *Molecular Physics*, **2018**, 116, 1328-1338	1.7	65
149	Calculated lanthanide contractions for molecular trihalides and fully hydrated ions: The contributions from relativity and 4f-shell hybridization. *Chemical Physics Letters*, **2006**, 429, 8-12	2.5	65
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147	Recent developments in the theory of f-element molecules. *Inorganica Chimica Acta*, **1987**, 139, 243-245	2.7	65
146	Relativistically parameterized extended hückel calculations. IX. An iterative version with applications to some xenon, thorium and uranium compounds. *Chemical Physics*, **1986**, 101, 355-369	2.3	64
145	Refitted tetrahedral covalent radii for solids. *Physical Review B*, **2012**, 85,	3.3	63
144	Scandium cycloheptanitride, ScN(7): a predicted high-energy molecule containing an [eta(7)-N(7)](3-) ligand. *Journal of the American Chemical Society*, **2001**, 123, 9700-1	16.4	63

143	REX calculations. 12. Iteration parameters for the 5f-element organometallics of thorium-neptunium. Geometries of thorium dioxide and uranyl ion revisited. *Inorganic Chemistry*, **1989**, 28, 1801-1805	5.1	62
142	Strong chemical bonds to gold. High level correlated relativistic results for diatomic AuBe+, AuC+, AuMg+, and AuSi+. *Chemical Physics Letters*, **1998**, 285, 398-403	2.5	61
141	Relativistic pseudopotential calculations on Xe2, RnXe, and Rn2: The van der Waals properties of radon **1998**, 66, 131-140		61
140	Relativistic pseudopotential calculation of bonding trends in XAum+n clusters (X = B□, Al□; n = 4□). *Chemical Physics Letters*, **1991**, 177, 103-106	2.5	61
139	Closed-shell interaction in silver and gold chlorides. *Journal of Chemical Physics*, **1998**, 109, 2339-2345	3.9	60
138	Calculated self-energy contributions for an ns valence electron using the multiple-commutator method. *Physical Review A*, **1999**, 59, 2707-2711	2.6	60
137	Molecular hydrogen tweezers: structure and mechanisms by neutron diffraction, NMR, and deuterium labeling studies in solid and solution. *Journal of the American Chemical Society*, **2011**, 133, 20245-57	16.4	59
136	Icosahedral WAu12: A Predicted Closed-Shell Species, Stabilized by Aurophilic Attraction and Relativity and in Accord with the 18-Electron Rule. *Angewandte Chemie*, **2002**, 114, 2278	3.6	58
135	The nuclear quadrupole moment of 14N obtained from finite-element MCHF calculationson N2+ (2p; 2P32) and N+ (2p2; 3P2 and 2p2; 1D2). *Chemical Physics Letters*, **1997**, 265, 60-64	2.5	57
134	Two-Dimensional, fully numerical molecular calculations. IV. hartree□ock□slater results on second-row diatomic molecules. *International Journal of Quantum Chemistry*, **1985**, 27, 601-612	2.1	57
133	Nuclear quadrupole moments of bismuth. *Physical Review Letters*, **2001**, 87, 133003	7.4	54
132	Ab initio study of bonding trends among the 14-electron diatomic systems: from B2 4- to F2 4+. *Molecular Physics*, **1989**, 67, 871-878	1.7	50
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130	An ab initio study of the aggregation of LAuX moleculesand [LAuL]+[XAuX]- ions. *Chemical Communications*, **1997**, 1111-1112	5.8	46
129	Aurophilic attraction: the additivity and the combination with hydrogen bonds. *Chemical Physics Letters*, **2003**, 370, 733-740	2.5	46
128	On bonding in transition-metal helide ions. *Molecular Physics*, **1984**, 52, 23-32	1.7	45
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124	Nuclear quadrupole moments of bromine and iodine from combined atomic and molecular data. *Physical Review A*, **2001**, 64,	2.6	44
123	Two-dimensional, fully numerical molecular calculations. *Molecular Physics*, **1987**, 60, 597-604	1.7	44
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117	Ab initio study of bonding trends 6. The X ? Y and X = Y = Z species containing phosphorus. *Molecular Physics*, **1990**, 70, 701-714	1.7	40
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115	A London-type formula for the dispersion interactions of endohedral A@B systems. *Physical Chemistry Chemical Physics*, **2007**, 9, 2954-8	3.6	38
114	Nuclear quadrupole moment of Hg201. *Physical Review A*, **2005**, 71,	2.6	38
113	A new, centered 32-electron system: the predicted [U@Si20]6□like isoelectronic series. *Chemical Science*, **2012**, 3, 2843	9.4	36
112	Coordination of pyridinethiols in gold(I) complexes. *Inorganic Chemistry*, **2007**, 46, 9954-60	5.1	36
111	Comparative calculations for the A-frame molecules [S(MPH3)2] (M=Cu, Ag, Au) at levels up to CCSD(T). *Chemical Physics Letters*, **2005**, 405, 148-152	2.5	36
110	One metal and forty nitrogens. Ab initio predictions for possible new high-energy pentazolides. *Inorganic Chemistry*, **2003**, 42, 8241-9	5.1	35
109	Calculations on indium and thallium cyclopentadienyls. Metal□metal interactions and possible new species. *Physical Chemistry Chemical Physics*, **1999**, 1, 3441-3444	3.6	35
108	Calculated properties of XeH2. *Chemical Physics Letters*, **1995**, 246, 239-244	2.5	35

107	Aurophilic attractions between a closed-shell molecule and a gold cluster. *Faraday Discussions*, **2011** , 152, 169-78; discussion 203-25	3.6	34
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99	The large range of uranyl bond lengths: ab initio calculations on simple uranium-oxygen clusters. *Inorganic Chemistry*, **1991**, 30, 3787-3788	5.1	31
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96	The importance of being tetrahedral: the cadmium pyramids CdN; N = 4, 10, 20, 35 and 56. *Physical Chemistry Chemical Physics*, **2004**, 6, 2907-2909	3.6	28
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92	Ab initio study of bonding trends among the 22-electron A?B?A systems: Evidence for O?O?O2+. *Chemical Physics Letters*, **1989**, 156, 337-340	2.5	27
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89	Darmstadtium carbonyl and carbide resemble platinum carbonyl and carbide. *Chemical Communications*, **2004**, 1982-3	5.8	25
88	On the Extreme Oxidation States of Iridium. *Chemistry - A European Journal*, **2015**, 21, 9468-73	4.8	24
87	Is the Lamb shift chemically significant?. *Chemical Physics Letters*, **2001**, 348, 497-500	2.5	24
86	Au22+ has bound excited states. *Chemical Physics Letters*, **2000**, 325, 225-231	2.5	24
85	Is Octavalent Pu(VIII) Possible? Mapping the Plutonium Oxyfluoride Series PuO(n)F(8-2n) (n = 0-4). *Inorganic Chemistry*, **2015**, 54, 8825-31	5.1	23
84	Formulations of the closed-shell interactions in endohedral systems. *Physical Chemistry Chemical Physics*, **2010**, 12, 6187-203	3.6	23
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58	The RTAM electronic bibliography, version 17.0, on relativistic theory of atoms and molecules. *Journal of Computational Chemistry*, **2013**, 34, 2667	3.5	16
57	Towards a 32-Electron Principle: Pu@Pb12 and Related Systems. *Angewandte Chemie*, **2007**, 119, 1449-1452	3.6	16
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