Paul Jerabek

List of Publications by Year
in descending order

49	1,650	304743	289244
papers	citations	22 h-index	40 g-index

57	57	57	1550
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Quantitative Assessment of Ligand Substituent Effects on Ïƒâ€•and Ï€â€Contributions to Feâ€”N Bonds in Spin Crossover Fe^{II}Complexes. Chemistry - A European Journal, 2022, 28, .	3.3	4
2	Modeling the thermodynamics of the FeTi hydrogenation under para-equilibrium: An ab-initio and experimental study. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2022, 77, 102426.	1.6	3
3	Magnesium- and intermetallic alloys-based hydrides for energy storage: modelling, synthesis and properties. Progress in Energy, 2022, 4, 032007.	10.9	29
4	Hydrogenation via a low energy mechanochemical approach: the MgB₂ case. JPhys Energy, 2021, 3, 044001.	5.3	4
5	Catalytic Asymmetric Fluorination of Copper Carbene Complexes: Preparative Advances and a Mechanistic Rationale. Chemistry - A European Journal, 2020, 26, 2509-2515.	3.3	24
6	Oganesson: Ein Edelgas, das weder edel noch ein Gas ist. Angewandte Chemie, 2020, 132, 23843-23848.	2.0	5
7	Quantitative and Chemically Intuitive Evaluation of the Nature of Mâ€”L Bonds in Paramagnetic Compounds: Application of EDAâ€NOCV Theory to Spin Crossover Complexes. Chemistry - A European Journal, 2020, 26, 13677-13685.	3.3	9
8	Oganesson: A Noble Gas Element That Is Neither Noble Nor a Gas. Angewandte Chemie - International Edition, 2020, 59, 23636-23640.	13.8	21
9	First-principles melting of krypton and xenon based on many-body relativistic coupled-cluster interaction potentials. Physical Review B, 2020, 101, .	3.2	15
10	Oganesson ist ein Halbleiter: Ãœber die relativitische BandlÃ¼ckenkontraktion in den schwersten Edelgasen. Angewandte Chemie, 2019, 131, 14398-14402.	2.0	8
11	Oganesson Is a Semiconductor: On the Relativistic Bandâ€Gap Narrowing in the Heaviest Nobleâ€Gas Solids. Angewandte Chemie - International Edition, 2019, 58, 14260-14264.	13.8	22
12	Solid Oganesson via a Many-Body Interaction Expansion Based on Relativistic Coupled-Cluster Theory and from Plane-Wave Relativistic Density Functional Theory. Journal of Physical Chemistry A, 2019, 123, 4201-4211.	2.5	23
13	Experimental FTIR and theoretical investigation of the molecular structure and vibrational spectra of acetanilide using DFT and dispersion correction to DFT. Journal of Theoretical and Computational Chemistry, 2019, 18, 1950009.	1.8	9
14	Ligands Based on Phosphineâ€Stabilized Aluminum(I), Boron(I), and Carbon(0). Chemistry - A European Journal, 2019, 25, 3068-3076.	3.3	6
15	Dative and electronâ€sharing bonding in transition metal compounds. Journal of Computational Chemistry, 2019, 40, 247-264.	3.3	74
16	Tipping the Balance between Ligand and Metal Protonation due to Relativistic Effects: Unusually High Proton Affinity in Gold(I) Pincer Complexes. Chemistry - A European Journal, 2018, 24, 6047-6051.	3.3	12
17	Electron and Nucleon Localization Functions of Oganesson: Approaching the Thomas-Fermi Limit. Physical Review Letters, 2018, 120, 053001.	7.8	79
18	A relativistic coupled-cluster interaction potential and rovibrational constants for the xenon dimer. Molecular Physics, 2018, 116, 1-8.	1.7	31

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19	The Lightâ€Driven Isomerization of Aqueous Nitrate: A Theoretical Perspective. ChemPhotoChem, 2018, 2, 725-733.	3.0	0
20	Suppressed Phosphine Dissociation by Polarization Effects on the Donorâ€“Acceptor Bonds in [Ni(PEt₃)_{4â€“n}(ECp*)_n] (E = Al, Ga). Inorganic Chemistry, 2018, 57, 12657-12664.	4.0	15
21	The Light-Driven Isomerization of Aqueous Nitrate: A Theoretical Perspective. ChemPhotoChem, 2018, 2, 702-702.	3.0	0
22	Static dipole polarizability of palladium from relativistic coupled-cluster theory. Physical Review A, 2018, 98, .	2.5	6
23	A Hundredâ€Yearâ€Old Experiment Reâ€evaluated: Accurate Abâ€…Initio Monteâ€…Carlo Simulations of the Melting of Radon. Angewandte Chemie - International Edition, 2018, 57, 9961-9964.	13.8	14
24	Ein hundert Jahre altes Experiment auf dem PrÃ¼fstand: hochgenaue Abâ€Initioâ€Monteâ€Carloâ€Schmelzsimulationen von Radon. Angewandte Chemie, 2018, 130, 10109-10113.	2.0	4
25	Influence of Relativistic Effects on Bonding Modes in M(II) Dinuclear Complexes (M = Au, Ag, and Cu). Inorganic Chemistry, 2017, 56, 14624-14631.	4.0	21
26	The Oxygenâ€Rich Beryllium Oxides BeO₄ and BeO₆. Angewandte Chemie - International Edition, 2016, 55, 10863-10867.	13.8	13
27	Understanding the F 1s NEXAFS Dichroism in Fluorinated Organic Semiconductors. Journal of Physical Chemistry C, 2016, 120, 12693-12705.	3.1	15
28	Znâ‹¯Zn interactions at nickel and palladium centers. Chemical Science, 2016, 7, 6413-6421.	7.4	30
29	Stepwise Synthesis of Siloxane-Substituted Oligoarsanes and Structural Investigation of Alkaline Earth Metal Derivatives. European Journal of Inorganic Chemistry, 2015, 2015, 3264-3273.	2.0	8
30	The Ïƒâ€Aromatic Clusters [Zn₃]⁺ and [Zn₂Cu]: Embryonic Brass. Angewandte Chemie - International Edition, 2015, 54, 4370-4374.	13.8	72
31	Dizinc Cation [Zn₂]²⁺ Trapped In A Homoleptic Metalloid Coordination Environment Stabilized by Dispersion Forces: [Zn₂(GaCp*)₆][BAr₄^F₂. Inorganic Chemistry, 2015, 54, 352-358.	4.0	21
32	Bonding analysis of telluroketones H2Aâ€‰=â€‰Te (A = C, Si, Ge). Journal of Molecular Modeling, 2014, 20, 2433.	1.8	3
33	Experimental Charge Density Study of a Silylone. Angewandte Chemie - International Edition, 2014, 53, 2766-2770.	13.8	115
34	A Novel Concept for the Synthesis of Multiply Doped Gold Clusters [(M@Au_nMâ€²_m)L_k]^{q+}. Angewandte Chemie - International Edition, 2014, 53, 4327-4331.	13.8	34
35	Comparative bonding analysis of N2 and P2 versus tetrahedral N4 and P4. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	27
36	Coinage Metals Binding as Main Group Elements: Structure and Bonding of the Carbene Complexes [TM(cAAC)₂] and [TM(cAAC)₂]⁺ (TM = Cu, Ag, Au). Journal of the American Chemical Society, 2014, 136, 17123-17135.	13.7	84

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37	Isolation of Neutral Mononuclear Copper Complexes Stabilized by Two Cyclic (Alkyl)(amino)carbenes. Journal of the American Chemical Society, 2014, 136, 6235-6238.	13.7	73
38	Humeâ€“Rothery Phase-Inspired Metal-Rich Molecules: Cluster Expansion of [Ni(ZnMe)₆(ZnCp*)₂] by Face Capping with Ni⁰(Î·⁶-toluene) and Ni^I(Î·⁵-Cp*). Inorganic Chemistry, 2014, 53, 10403-10411.	4.0	15
39	Isolation of Neutral Monoâ€•and Dinuclear Gold Complexes of Cyclic (Alkyl)(amino)carbenes. Angewandte Chemie - International Edition, 2013, 52, 8964-8967.	13.8	119
40	Reductive elimination: a pathway to low-valent aluminium species. Chemical Communications, 2013, 49, 2858.	4.1	94
41	Nearly Degenerate Isomers of C(BH)₂: Cumulene, Carbene, or Carbone?. Chemistry - A European Journal, 2013, 19, 15941-15954.	3.3	25
42	The Organozinc Rich Compounds [Cp*M(ZnR)₅] (M = Fe, Ru; R = Cp*, Me, Cl, Br). Inorganic Chemistry, 2013, 52, 7152-7160.	4.0	11
43	Structures and energies of C4S4q (q=+1, 0, â^'1) isomers. A theoretical study. International Journal of Mass Spectrometry, 2013, 354-355, 342-345.	1.5	0
44	[3+2] Fragmentation of an [RP₅Cl]⁺ Cage Cation Induced by an Nâ€Heterocyclic Carbene. Angewandte Chemie - International Edition, 2013, 52, 11078-11082.	13.8	49
45	A Crystalline Singlet Phosphinonitrene: A Nitrogen Atomâ€“Transfer Agent. Science, 2012, 337, 1526-1528.	12.6	148
46	Ligandâ€Stabilized [P₄]²⁺ Cations. Angewandte Chemie - International Edition, 2012, 51, 2964-2967.	13.8	67
47	Oligonuclear Molecular Models of Intermetallic Phases: A Case Study on [Pd₂Zn₆Ga₂(Cp*)₅(CH₃)₃]. Chemistry - A European Journal, 2012, 18, 4909-4915.	3.3	16
48	Hunting dimers. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	6
49	The Rich Chemistry of [Zn₂Cp*₂]: Trapping Three Different Types of Zinc Ligands in the PdZn₇Complex [Pd(ZnCp*)₄(ZnMe)₂{Zn(tmeda)}]. Inorganic Chemistry, 2011, 50, 10486-10492.	4.0	26