Philippe F Weck

List of Publications by Year in Descending Order

92 papers	1,495 citations	22 h-index	33 g-index
99 ext. papers	1,671 ext. citations	4.2 avg, IF	4.69 L-index

#	Paper	IF	Citations
92	Effect of Excess Mg to Control Corrosion in Molten MgCl2 and KCl Eutectic Salt Mixture. *Corrosion Science*, **2021**, 109914	6.8	2
91	Thermodynamic properties of metaschoepite predicted from density functional perturbation theory. *Chemical Physics Letters*, **2020**, 757, 137878	2.5	0
90	Shock compression of vanadium at extremes: Theory and experiment. *Physical Review B*, **2020**, 102,	3.3	5
89	Strain-controlled magnetic ordering in 2D carbon metamaterials. *Carbon*, **2020**, 161, 219-223	10.4	4
88	Molecular dynamics simulation of zirconium tungstate amorphization and the amorphous-crystalline interface. *Journal of Physics Condensed Matter*, **2020**, 32, 085401	1.8	3
87	Radionuclide incorporation in negative thermal expansion □Zr(WO4)2: A density functional theory study. *Chemical Physics Letters*, **2020**, 744, 137172	2.5	1
86	High-precision equation of state data for TiO2: A structural analog of SiO2. *Physical Review B*, **2020**, 102,	3.3	4
85	Crystal and Electronic Structures of ANaIO Periodate Double Perovskites (A = Sr, Ca, Ba): Candidate Wasteforms for I-129 Immobilization. *Inorganic Chemistry*, **2020**, 59, 18407-18419	5.1	3
84	Auger electron emission in proton-induced interactions in living matter: A TILDA-V Monte Carlo tracking. *X-Ray Spectrometry*, **2020**, 49, 95-98	0.9	
83	Shock compression of niobium from first-principles. *Journal of Applied Physics*, **2019**, 125, 245905	2.5	6
82	Zirconium chloride molecular species: combining electron impact mass spectrometry and first principles calculations. *SN Applied Sciences*, **2019**, 1, 1	1.8	1
81	Elucidating Structure□Spectral Property Relationships of Negative Thermal Expansion Zr2(WO4)(PO4)2: A First-Principles Study with Experimental Validation. *Journal of Physical Chemistry C*, **2019**, 123, 21607-21616	3.8	
80	Structure-thermodynamics relationship of schoepite from first-principles. *Physical Chemistry Chemical Physics*, **2019**, 21, 25569-25576	3.6	3
79	Shock compression of strongly correlated oxides: A liquid-regime equation of state for cerium(IV) oxide. *Physical Review B*, **2018**, 97,	3.3	10
78	Phosphorus Dimerization in Gallium Phosphide at High Pressure. *Inorganic Chemistry*, **2018**, 57, 2432-2437	5.1	7
77	Assessing exchange-correlation functionals for elasticity and thermodynamics of □ZrW2O8: A density functional perturbation theory study. *Chemical Physics Letters*, **2018**, 698, 195-199	2.5	6
76	Reverse-martensitic hcp-to-fcc transformation in technetium under shock compression. *Journal of Applied Physics*, **2018**, 124, 035903	2.5	5

75	Lattice dynamics and thermomechanical properties of zirconium(IV) chloride: Evidence for low-temperature negative thermal expansion. *Chemical Physics Letters*, **2018**, 691, 98-102	2.5	5
74	First-Principles Structural, Mechanical, and Thermodynamic Calculations of the Negative Thermal Expansion Compound Zr(WO)(PO). *ACS Omega*, **2018**, 3, 15780-15788	3.9	7
73	High-pressure-assisted X-ray-induced damage as a new route for chemical and structural synthesis. *Physical Chemistry Chemical Physics*, **2018**, 20, 18949-18956	3.6	9
72	Infrared and Raman spectroscopy of □ZrW2O8: A comprehensive density functional perturbation theory and experimental study. *Journal of Raman Spectroscopy*, **2018**, 49, 1373-1384	2.3	8
71	Zirconium tetrachloride revisited. *Acta Crystallographica Section C, Structural Chemistry*, **2018**, 74, 307-311	0.8	2
70	Model representations of kerogen structures: An insight from density functional theory calculations and spectroscopic measurements. *Scientific Reports*, **2017**, 7, 7068	4.9	13
69	Density Functional Analysis of Fluorite-Structured (Ce, Zr)O2/CeO2 Interfaces. *Journal of Physical Chemistry C*, **2017**, 121, 14678-14687	3.8	7
68	Monte Carlo simulation of proton track structure in biological matter. *European Physical Journal D*, **2017**, 71, 1	1.3	15
67	Assessing Hubbard-corrected AM05+U and PBEsol+U density functionals for strongly correlated oxides CeO and CeO. *Physical Chemistry Chemical Physics*, **2016**, 18, 26816-26826	3.6	19
66	Technetium incorporation in scheelite: insights from first-principles. *Dalton Transactions*, **2016**, 45, 18171-18176	4.3	6
65	Energetics of Sn2+ isomorphic substitution into hydroxylapatite: first-principles predictions. *RSC Advances*, **2016**, 6, 107286-107292	3.7	0
64	van der Waals forces and confinement in carbon nanopores: Interaction between CH4, COOH, NH3, OH, SH and single-walled carbon nanotubes. *Chemical Physics Letters*, **2016**, 652, 22-26	2.5	4
63	Uncloaking the Thermodynamics of the Studtite to Metastudtite Shear-Induced Transformation. *Journal of Physical Chemistry C*, **2016**, 120, 16553-16560	3.8	28
62	Low energy electrons and swift ion track structure in PADC. *Radiation Physics and Chemistry*, **2015**, 115, 36-42	2.5	9
61	Relationship between crystal structure and thermo-mechanical properties of kaolinite clay: beyond standard density functional theory. *Dalton Transactions*, **2015**, 44, 12550-60	4.3	26
60	Thermodynamics of technetium: reconciling theory and experiment using density functional perturbation analysis. *Dalton Transactions*, **2015**, 44, 12735-42	4.3	11
59	Dehydration of uranyl nitrate hexahydrate to uranyl nitrate trihydrate under ambient conditions as observed via dynamic infrared reflectance spectroscopy **2015**,		3
58	Interaction of cesium adatoms with free-standing graphene and graphene-veiled SiO2 surfaces. *RSC Advances*, **2015**, 5, 38623-38629	3.7	2

57	Mechanical properties of zirconium alloys and zirconium hydrides predicted from density functional perturbation theory. *Dalton Transactions*, **2015**, 44, 18769-79	4.3	37
56	On the mechanical stability of uranyl peroxide hydrates: implications for nuclear fuel degradation. *RSC Advances*, **2015**, 5, 79090-79097	3.7	41
55	Electron- and proton-induced ionization of pyrimidine. *European Physical Journal D*, **2015**, 69, 1	1.3	7
54	Time-Resolved Infrared Reflectance Studies of the Dehydration-Induced Transformation of Uranyl Nitrate Hexahydrate to the Trihydrate Form. *Journal of Physical Chemistry A*, **2015**, 119, 9996-10006	2.8	22
53	Speciation of technetium peroxo complexes in sulfuric acid revisited. *Journal of Radioanalytical and Nuclear Chemistry*, **2015**, 303, 1163-1167	1.5	2
52	First-principles study of anhydrite, polyhalite and carnallite. *Chemical Physics Letters*, **2014**, 594, 1-5	2.5	15
51	Layered uranium(VI) hydroxides: structural and thermodynamic properties of dehydrated schoepite □UO(□OH)□ *Dalton Transactions*, **2014**, 43, 17191-9	4.3	33
50	Solar Energy Storage in Phase Change Materials: First-Principles Thermodynamic Modeling of Magnesium Chloride Hydrates. *Journal of Physical Chemistry C*, **2014**, 118, 4618-4625	3.8	38
49	Theoretical and experimental quantification of doubly and singly differential cross sections for electron-induced ionization of isolated tetrahydrofuran molecules. *European Physical Journal D*, **2014**, 68, 1	1.3	4
48	Magic numbers in small iron clusters: A first-principles study. *Chemical Physics Letters*, **2014**, 613, 59-63	2.5	23
47	Nuclear forward scattering and first-principles studies of the iron oxide phase Fe4O5. *Physical Review B*, **2014**, 90,	3.3	7
46	First-Principles and Kinetic Monte Carlo Simulation Studies of the Reactivity of Tc(0001), MoTc(111) and MoTc(110) Surfaces. *Journal of the Electrochemical Society*, **2014**, 161, C83-C88	3.9	10
45	□Technetium dichloride: solid-state modulated structure, electronic structure, and physical properties. *Journal of the American Chemical Society*, **2013**, 135, 15955-62	16.4	7
44	Semiconducting layered technetium dichalcogenides: insights from first-principles. *Dalton Transactions*, **2013**, 42, 15288-95	4.3	17
43	Reactivity of HTcO(4) with methanol in sulfuric acid: Tc-sulfate complexes revealed by XAFS spectroscopy and first principles calculations. *Dalton Transactions*, **2013**, 42, 4348-52	4.3	22
42	Diperoxo Pertechnetic Acid Characterized by Spectroscopic and Quantum Chemical Studies. *European Journal of Inorganic Chemistry*, **2013**, 2013, 4595-4600	2.3	4
41	Trivalent actinide and lanthanide complexation of 5,6-dialkyl-2,6-bis(1,2,4-triazin-3-yl)pyridine (RBTP; R = H, Me, Et) derivatives: a combined experimental and first-principles study. *Inorganic Chemistry*, **2013**, 52, 761-76	5.1	17
40	X-ray Crystallographic and First-Principles Theoretical Studies of K2[TcOCl5] and UV/Vis Investigation of the [TcOCl5]2□and [TcOCl4]□Ions. *European Journal of Inorganic Chemistry*, **2013**, 2013, 1097-1104	2.3	1

39	On the role of strong electron correlations in the surface properties and chemistry of uranium dioxide. *Dalton Transactions*, **2013**, 42, 4570-8	4.3	31
38	Worker exposure for at-reactor management of spent nuclear fuel. *Radiation Protection Dosimetry*, **2013**, 156, 386-93	0.9	0
37	First evidence for the formation of technetium oxosulfide complexes: synthesis, structure and characterization. *Dalton Transactions*, **2012**, 41, 6291-8	4.3	11
36	Structures of uranyl peroxide hydrates: a first-principles study of studtite and metastudtite. *Dalton Transactions*, **2012**, 41, 9748-52	4.3	50
35	Crystal and electronic structures of neptunium nitrides synthesized using a fluoride route. *Journal of the American Chemical Society*, **2012**, 134, 3111-9	16.4	14
34	On the structure of □molybdenum dichloride. *Inorganic Chemistry*, **2012**, 51, 4965-71	5.1	2
33	□Technetium trichloride: formation, structure, and first-principles calculations. *Inorganic Chemistry*, **2012**, 51, 4915-7	5.1	16
32	Quantum-Mechanical Contributions to Numerical Simulations of Charged Particle Transport at the DNA Scale **2012**, 263-289		6
31	Ion-induced ionization and capture cross sections for DNA nucleobases impacted by light ions. *Journal of Physics: Conference Series*, **2012**, 388, 102004	0.3	
30	Ionization and capture in water: a multi-differential cross sections study. *Journal of Physics: Conference Series*, **2012**, 388, 102003	0.3	1
29	Chemical bonding and aromaticity in trinuclear transition-metal halide clusters. *Inorganic Chemistry*, **2011**, 50, 1039-46	5.1	22
28	Nanoconfinement effects on the reversibility of hydrogen storage in ammonia borane: a first-principles study. *Journal of Chemical Physics*, **2011**, 134, 214501	3.9	14
27	Discovery of the recoverable high-pressure iron oxide Fe4O5. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 17281-5	11.5	94
26	Technetium dichloride: a new binary halide containing metal-metal multiple bonds. *Journal of the American Chemical Society*, **2011**, 133, 8814-7	16.4	27
25	One-dimensional uranium-organic coordination polymers: crystal and electronic structures of uranyl-diacetohydroxamate. *Dalton Transactions*, **2011**, 40, 6007-11	4.3	16
24	Interplay between structure, stoichiometry and properties of technetium nitrides. *Dalton Transactions*, **2011**, 40, 6738-44	4.3	18
23	Density functional analysis of the trigonal uranyl equatorial coordination in hexahomotrioxacalix[3]arene-based macrocyclic complexes. *Inorganic Chemistry*, **2010**, 49, 1465-70	5.1	14
22	Structural and magnetic properties of Tcn@C60 endohedral metalofullerenes: First-principles predictions. *Physical Review B*, **2010**, 81,	3.3	18

21	Synthesis and structure of technetium trichloride. *Journal of the American Chemical Society*, **2010**, 132, 15864-5	16.4	27
20	Structural and electronic trends in rare-earth technetate pyrochlores. *Dalton Transactions*, **2010**, 39, 7207-10	4.3	12
19	Structural studies of technetium-zirconium alloys by X-ray diffraction, high-resolution electron microscopy, and first-principles calculations. *Inorganic Chemistry*, **2010**, 49, 1433-8	5.1	13
18	Speciation of heptavalent technetium in sulfuric acid: structural and spectroscopic studies. *Dalton Transactions*, **2010**, 39, 8616-9	4.3	28
17	First-principles study of the hexahalogenotechnetate(IV) ions TcX62- [X = Cl, Br]. *Chemical Physics Letters*, **2010**, 487, 190-193	2.5	6
16	Organic cyclic difluoramino-nitramines: infrared and Raman spectroscopy of 3,3,7,7-tetrakis(difluoramino)octahydro 1,5-dinitro-1,5-diazocine (HNFX). *Journal of Raman Spectroscopy*, **2009**, 40, 964-971	2.3	6
15	Technetium(IV) halides predicted from first-principles. *Inorganic Chemistry*, **2009**, 48, 6555-8	5.1	22
14	Synthesis, structure, and first-principles calculations of [TcBr2(PMe3)4] and [Tc2Br4(PMe3)4] complexes. *Dalton Transactions*, **2009**, 10338-42	4.3	19
13	Structural evolution and properties of subnanometer Tc(n) (n = 2-15) clusters. *Physical Chemistry Chemical Physics*, **2009**, 11, 10003-8	3.6	15
12	Raman spectroscopic study of cyclopentane at high pressure. *Journal of Chemical Physics*, **2009**, 130, 204505	3.9	5
11	Dimer-induced stabilization of H adsorbate cluster on BN(0001) surface. *Physical Chemistry Chemical Physics*, **2008**, 10, 5184-7	3.6	10
10	Nanoscale building blocks for the development of novel proton exchange membrane fuel cells. *Journal of Physical Chemistry B*, **2008**, 112, 3283-6	3.4	33
9	High-pressure studies of 1,3,5,7-cyclooctatetraene: experiment and theory. *Journal of Physical Chemistry A*, **2008**, 112, 11501-7	2.8	11
8	Hydrogenation of single-wall carbon nanotubes using polyamine reagents: combined experimental and theoretical study. *Journal of the American Chemical Society*, **2008**, 130, 2296-303	16.4	48
7	Mechanism of fullerene hydrogenation by polyamines: Ab initio density functional calculations. *Physical Review B*, **2008**, 78,	3.3	28
6	Evolution of Small Ti Clusters and the Dissociative Chemisorption of H2on Ti. *Journal of Physical Chemistry C*, **2007**, 111, 7494-7500	3.8	54
5	Designing carbon nanoframeworks tailored for hydrogen storage. *Chemical Physics Letters*, **2007**, 439, 354-359	2.5	17
4	First-principles study of single-crystal uranium mono- and dinitride. *Chemical Physics Letters*, **2007**, 443, 82-86	2.5	45

3	Pressure-driven phase transitions in NaBH4: theory and experiments. *Journal of Physical Chemistry B*, **2007**, 111, 13873-6	3.4	32
2	Computational study of hydrogen storage in organometallic compounds. *Journal of Chemical Physics*, **2007**, 126, 094703	3.9	85
1	Importance of long-range interactions in chemical reactions at cold and ultracold temperatures. *International Reviews in Physical Chemistry*, **2006**, 25, 283-311	7	83