Piotr Kowalski

List of Publications by Year in Descending Order

89 papers	2,158 citations	25 h-index	43 g-index
99 ext. papers	2,491 ext. citations	4.4 avg, IF	5.3 L-index

#	Paper	IF	Citations
89	Water structures on Pb(100) and (111) surface studied with the Interface force field. *Applied Surface Science*, **2022**, 589, 152838	6.7	1
88	Gamma radiolytic stability of the novel modified diglycolamide 2,2Q-oxybis(,-didecylpropanamide) (mTDDGA) for grouped actinide extraction.. *RSC Advances*, **2022**, 12, 12416-12426	3.7	1
87	Monazite-Type SmPO4 as Potential Nuclear Waste Form: Insights into Radiation Effects from Ion-Beam Irradiation and Atomistic Simulations. *Materials*, **2022**, 15, 3434	3.5	0
86	Pyrochlore Compounds From Atomistic Simulations. *Frontiers in Chemistry*, **2021**, 9, 733321	5	0
85	The Structure of the Electric Double Layer of the Protic Ionic Liquid [Dema][TfO] Analyzed by Atomic Force Spectroscopy. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	1
84	Electrode and Electrolyte Materials From Atomistic Simulations: Properties of LixFEPO4 Electrode and Zircon-Based Ionic Conductors. *Frontiers in Energy Research*, **2021**, 9,	3.8	1
83	Properties of irradiated sodium borosilicate glasses from experiment and atomistic simulations. *Journal of the American Ceramic Society*, **2021**, 104, 4479-4491	3.8	1
82	Achieving and Stabilizing Uranyl Bending via Physical Pressure. *Inorganic Chemistry*, **2021**, 60, 8419-8422	5.1	0
81	Ion distribution models for defect fluorite ZrO2 - AO1.5 (A = Ln, Y) solid solutions: I. Relationship between lattice parameter and composition. *Acta Materialia*, **2021**, 202, 99-111	8.4	10
80	Tilting and Distortion in Rutile-Related Mixed Metal Ternary Uranium Oxides: A Structural, Spectroscopic, and Theoretical Investigation. *Inorganic Chemistry*, **2021**, 60, 2246-2260	5.1	5
79	Properties of the Pt(111)/electrolyte electrochemical interface studied with a hybrid DFT-solvation approach. *Journal of Physics Condensed Matter*, **2021**, 33,	1.8	6
78	Deprotonation and Cation Adsorption on the NiOOH/Water Interface: A Grand-Canonical First-Principles Investigation. *Electrochimica Acta*, **2021**, 139253	6.7	1
77	Research for the Safe Management of Nuclear Waste at Forschungszentrum J□ch: Materials Chemistry and Solid Solution Aspects. *Advanced Engineering Materials*, **2020**, 22, 1901417	3.5	6
76	Modeling of Nuclear Waste Forms: State-of-the-Art and Perspectives. *MRS Advances*, **2020**, 5, 213-222	0.7	
75	Insights into the fabrication and structure of plutonium pyrochlores. *Journal of Materials Chemistry A*, **2020**, 8, 2387-2403	13	10
74	The +2 oxidation state of Cr incorporated into the crystal lattice of UO2. *Communications Materials*, **2020**, 1,	6	6
73	Formation enthalpy of Ln2B2O7-type (B=Ti,Sn,Hf,Zr) compounds. *Scripta Materialia*, **2020**, 189, 7-10	5.6	6

72	Elastic and thermal parameters of lanthanide-orthophosphate (LnPO4) ceramics from atomistic simulations. *Journal of the European Ceramic Society*, **2019**, 39, 4264-4274	6	1
71	Application of layered double hydroxides for 99Tc remediation. *Applied Clay Science*, **2019**, 176, 1-10	5.2	7
70	Rare-Earth Orthophosphates From Atomistic Simulations. *Frontiers in Chemistry*, **2019**, 7, 197	5	9
69	Controlling Oxygen Defect Formation and Its Effect on Reversible Symmetry Lowering and Disorder-to-Order Phase Transformations in Nonstoichiometric Ternary Uranium Oxides. *Inorganic Chemistry*, **2019**, 58, 6143-6154	5.1	9
68	Unprecedented Inversion of Selectivity and Extraordinary Difference in the Complexation of Trivalent f Elements by Diastereomers of a Methylated Diglycolamide. *Chemistry - A European Journal*, **2019**, 25, 5507-5513	4.8	14
67	Americium incorporation into studtite: a theoretical and experimental study. *Dalton Transactions*, **2019**, 48, 13057-13063	4.3	3
66	An experimental calorimetric and a DFT + U study of the thermodynamic properties of Cs4UO24WO5W2O8O2 and Cs4[UO27WO53O3]. *Journal of Chemical Thermodynamics*, **2019**, 139, 105873	2.9	2
65	Dehydration of the Uranyl Peroxide Studtite, [UO(□O)(HO)]□2HO, Affords a Drastic Change in the Electronic Structure: A Combined X-ray Spectroscopic and Theoretical Analysis. *Inorganic Chemistry*, **2018**, 57, 1735-1743	5.1	21
64	Unexpected Crystallographic Phase Transformation in Nonstoichiometric SrUO: Reversible Oxygen Defect Ordering and Symmetry Lowering with Increasing Temperature. *Inorganic Chemistry*, **2018**, 57, 5948-5958	5.1	13
63	Uptake of 226Ra in cementitious systems: A complementary solution chemistry and atomistic simulation study. *Applied Geochemistry*, **2018**, 96, 204-216	3.5	13
62	Trends in the valence band electronic structures of mixed uranium oxides. *Chemical Communications*, **2018**, 54, 9757-9760	5.8	15
61	Energetics of defects formation and oxygen migration in pyrochlore compounds from first principles calculations. *Journal of Nuclear Materials*, **2018**, 505, 255-261	3.3	15
60	Boron Isotope Fractionation Among Vapor□iquids□olids□Melts: Experiments and Atomistic Modeling. *Advances in Isotope Geochemistry*, **2018**, 33-69	1.2	14
59	A Spectroscopic and Computational Study of Cm Incorporation in Lanthanide Phosphate Rhabdophane (LnPO□0.67HO) and Monazite (LnPO). *Inorganic Chemistry*, **2018**, 57, 6252-6265	5.1	11
58	Probing structural homogeneity of La 1-x Gd x PO 4 monazite-type solid solutions by combined spectroscopic and computational studies. *Journal of Nuclear Materials*, **2017**, 486, 148-157	3.3	18
57	Cation-Dependent Structural Evolution in A2Th(TVO4)2(A = Li, Na, K, Rb, Cs; T = P and As) Series. *Crystal Growth and Design*, **2017**, 17, 1339-1346	3.5	7
56	Towards Reliable Modeling of Challengingf Electrons Bearing Materials: Experience from Modeling of Nuclear Materials. *MRS Advances*, **2017**, 2, 491-497	0.7	7
55	Composition dependent order-disorder transition in Nd Zr1□02□.5 pyrochlores: A combined structural, calorimetric and ab initio modeling study. *Acta Materialia*, **2017**, 125, 166-176	8.4	26

54	Large Scale Simulation of Nuclear Waste Materials. *Energy Procedia*, **2017**, 127, 416-424	2.3	8
53	New insights into phosphate based materials for the immobilisation of actinides. *Radiochimica Acta*, **2017**, 105, 961-984	1.9	37
52	Pressure Distortion of the H2He Collision-induced Absorption at the Photosphere of Cool White Dwarf Stars. *Astrophysical Journal*, **2017**, 848, 36	4.7	18
51	Heat capacities of xenotime-type ceramics: An accurate ab initio prediction. *Journal of Nuclear Materials*, **2017**, 494, 172-181	3.3	12
50	Simulation of ceramic materials relevant for nuclear waste management: Case of La1Eu PO4 solid solution. *Nuclear Instruments & Methods in Physics Research B*, **2017**, 393, 68-72	1.2	13
49	Atomistic modeling and experimental studies of radiation damage in monazite-type LaPO4 ceramics. *Nuclear Instruments & Methods in Physics Research B*, **2017**, 393, 54-58	1.2	21
48	Thermochemistry of La1LnxPO4-monazites (Ln= Gd, Eu). *Journal of Chemical Thermodynamics*, **2017**, 105, 396-403	2.9	31
47	Experimental and Theoretical Evidence for Surface-Induced Carbon and Nitrogen Fractionation during Diamond Crystallization at High Temperatures and High Pressures. *Crystals*, **2017**, 7, 190	2.3	6
46	Nonstoichiometry in Strontium Uranium Oxide: Understanding the Rhombohedral-Orthorhombic Transition in SrUO4. *Inorganic Chemistry*, **2016**, 55, 9329-34	5.1	18
45	Atomistic Simulations of Ceramic Materials Relevant for Nuclear Waste Management: Cases of Monazlte and Pyrochlore. *Ceramic Transactions*, **2016**, 165-175	0.1	10
44	DFT+U as a reliable method for efficient ab initio calculations of nuclear materials. *Progress in Nuclear Energy*, **2016**, 92, 142-146	2.3	23
43	Adsorbate-induced lifting of substrate relaxation is a general mechanism governing titania surface chemistry. *Nature Communications*, **2016**, 7, 12888	17.4	18
42	Giant Volume Change and Topological Gaps in Temperature- and Pressure-Induced Phase Transitions: Experimental and Computational Study of ThMo2 O8. *Chemistry - A European Journal*, **2016**, 22, 946-58	4.8	6
41	Relationship between the thermodynamic excess properties of mixing and the elastic moduli in the monazite-type ceramics. *Journal of the European Ceramic Society*, **2016**, 36, 2093-2096	6	28
40	Feasible and Reliable AB Initio Approach to Computation of Materials Relevant for Nuclear Waste Management. *Ceramic Transactions*, **2016**, 205-217	0.1	6
39	Defect formation energies in A2B2O7 pyrochlores. *Scripta Materialia*, **2015**, 107, 18-21	5.6	53
38	Heat capacities of lanthanide and actinide monazite-type ceramics. *Journal of Nuclear Materials*, **2015**, 464, 147-154	3.3	31
37	Performance of DFT+U method for prediction of structural and thermodynamic parameters of monazite-type ceramics. *Journal of Computational Chemistry*, **2014**, 35, 1339-46	3.5	43

36	Ab initio calculation of excess properties of La1−x(Ln,An)xPO4 solid solutions. *Journal of Solid State Chemistry*, **2014**, 220, 137-141	3.3	45
35	Benchmarking the DFT+U method for thermochemical calculations of uranium molecular compounds and solids. *Journal of Physical Chemistry A*, **2014**, 118, 11797-810	2.8	49
34	Theoretical Approaches to Structure and Spectroscopy of Earth Materials. *Reviews in Mineralogy and Geochemistry*, **2014**, 78, 691-743	7.1	33
33	Highly distorted uranyl ion coordination and one/two-dimensional structural relationship in the Ba2[UO2(TO4)2] (T = P, As) system: an experimental and computational study. *Inorganic Chemistry*, **2014**, 53, 7650-60	5.1	17
32	Polarimetry as a tool to find and characterise habitable planets orbiting white dwarfs. *Proceedings of the International Astronomical Union*, **2014**, 10, 325-332	0.1	2
31	Infrared absorption of dense helium and its importance in the atmospheres of cool white dwarfs. *Astronomy and Astrophysics*, **2014**, 566, L8	5.1	10
30	A NEW OCCURRENCE OF THE BOROSILICATE SERENDIBITE IN TOURMALINE-BEARING CALC-SILICATE ROCKS, PORTAGE-DU-FORT MARBLE, GRENVILLE PROVINCE, QUEBEC: EVOLUTION OF BORON ISOTOPE AND TOURMALINE COMPOSITIONS IN A METAMORPHIC CONTEXT. *Canadian Mineralogist*, **2014**, 52, 595-616	0.7	4
29	17. Theoretical Approaches to Structure and Spectroscopy of Earth Materials **2014**, 691-744		1
28	NEAR-UV ABSORPTION IN VERY COOL DA WHITE DWARFS. *Astrophysical Journal*, **2014**, 790, 50	4.7	6
27	Gaiaphotometry for white dwarfs. *Astronomy and Astrophysics*, **2014**, 565, A11	5.1	40
26	Vibrational properties of silica species in MgO–SiO2 glasses obtained from ab initio molecular dynamics. *Chemical Geology*, **2013**, 346, 22-33	4.2	23
25	Boron isotopic composition of tourmaline, prismatine, and grandidierite from granulite facies paragneisses in the Larsemann Hills, Prydz Bay, East Antarctica: Evidence for a non-marine evaporite source. *Geochimica Et Cosmochimica Acta*, **2013**, 123, 261-283	5.5	30
24	Ab initio prediction of equilibrium boron isotope fractionation between minerals and aqueous fluids at high P and T. *Geochimica Et Cosmochimica Acta*, **2013**, 101, 285-301	5.5	64
23	11–12 Gyr old white dwarfs 30 pc away. *Monthly Notices of the Royal Astronomical Society: Letters*, **2012**, 423, L132-L136	4.3	21
22	THE SPECTRUM OF THE RECYCLED PSR J0437−4715 AND ITS WHITE DWARF COMPANION. *Astrophysical Journal*, **2012**, 746, 6	4.7	51
21	Vibrational mode frequencies of H4SiO4, D4SiO4, H6Si2O7, and H6Si3O9 in aqueous environment, obtained from ab initio molecular dynamics. *Journal of Chemical Physics*, **2012**, 137, 164506	3.9	14
20	THE HABITABILITY AND DETECTION OF EARTH-LIKE PLANETS ORBITING COOL WHITE DWARFS. *Astrophysical Journal Letters*, **2012**, 757, L15	7.9	35
19	Prediction of equilibrium Li isotope fractionation between minerals and aqueous solutions at high P and T: An efficient ab initio approach. *Geochimica Et Cosmochimica Acta*, **2011**, 75, 6112-6123	5.5	55

18	Ideal, defective, and gold-promoted rutile TiO2(110) surfaces interacting with CO, H2, and H2O: Structures, energies, thermodynamics, and dynamics from PBE+U. *Physical Review B*, **2011**, 84,	3.3	51
17	Charge localization dynamics induced by oxygen vacancies on the TiO2(110) surface. *Physical Review Letters*, **2010**, 105, 146405	7.4	178
16	VISITORS FROM THE HALO: 11 Gyr OLD WHITE DWARFS IN THE SOLAR NEIGHBORHOOD. *Astrophysical Journal Letters*, **2010**, 715, L21-L25	7.9	25
15	The origin of peculiar molecular bands in cool DQ white dwarfs. *Astronomy and Astrophysics*, **2010**, 519, L8	5.1	25
14	A LARGE STELLAR EVOLUTION DATABASE FOR POPULATION SYNTHESIS STUDIES. VI. WHITE DWARF COOLING SEQUENCES. *Astrophysical Journal*, **2010**, 716, 1241-1251	4.7	79
13	A NEAR-INFRARED SPECTROSCOPIC SURVEY OF COOL WHITE DWARFS IN THE SLOAN DIGITAL SKY SURVEY. *Astronomical Journal*, **2009**, 138, 102-109	4.9	13
12	Formation of weakly bound, ordered adlayers of CO on rutile TiO2(110): a combined experimental and theoretical study. *Journal of Chemical Physics*, **2009**, 130, 144703	3.9	38
11	Composition, structure, and stability of the rutile TiO2(110) surface: Oxygen depletion, hydroxylation, hydrogen migration, and water adsorption. *Physical Review B*, **2009**, 79,	3.3	203
10	SPITZEROBSERVATIONS OF THE OLDEST WHITE DWARFS IN THE SOLAR NEIGHBORHOOD. *Astrophysical Journal*, **2009**, 696, 2094-2103	4.7	24
9	A NEARBY OLD HALO WHITE DWARF CANDIDATE FROM THE SLOAN DIGITAL SKY SURVEY. *Astronomical Journal*, **2008**, 136, 76-82	4.9	23
8	The First Mid-Infrared Spectra of Cool White Dwarfs. *Astrophysical Journal*, **2008**, 678, 1298-1303	4.7	10
7	Equation of state and optical properties of warm dense helium. *Physical Review B*, **2007**, 76,	3.3	54
6	He Conductivity in Cool White Dwarf Atmospheres. *Astrophysics and Space Science*, **2007**, 307, 273-277	1.6	5
5	White dwarf atmosphere models with Ly-alpha opacity in the analysis of the white dwarf cooling sequence of NGC 6397. *Astronomy and Astrophysics*, **2007**, 474, 491-494	5.1	12
4	On the Dissociation Equilibrium of H2in Very Cool, Helium-rich White Dwarf Atmospheres. *Astrophysical Journal*, **2006**, 641, 488-493	4.7	24
3	Found: The Missing Blue Opacity in Atmosphere Models of Cool Hydrogen White Dwarfs. *Astrophysical Journal*, **2006**, 651, L137-L140	4.7	209
2	The Pseudocontinuum Bound-Free Opacity of Hydrogen and Its Importance in Cool White Dwarf Atmospheres. *Astrophysical Journal*, **2006**, 651, 1120-1125	4.7	11
1	Radiative Transfer in the Refractive Atmospheres of Very Cool White Dwarfs. *Astrophysical Journal*, **2004**, 607, 970-981	4.7	31