Ville R I Kaila

List of Publications by Year in Descending Order

86 papers	2,906 citations	32 h-index	51 g-index
91 ext. papers	3,527 ext. citations	10.5 avg, IF	5.91 L-index

#	Paper	IF	Citations
86	Molecular Principles of Redox-Coupled Protonation Dynamics in Photosystem II.. *Journal of the American Chemical Society*, **2022**,	16.4	6
85	Extended conformational states dominate the Hsp90 chaperone dynamics. *Journal of Biological Chemistry*, **2022**, 102101	5.4	1
84	Design of buried charged networks in artificial proteins. *Nature Communications*, **2021**, 12, 1895	17.4	5
83	Molecular strain in the active/deactive-transition modulates domain coupling in respiratory complex I. *Biochimica Et Biophysica Acta - Bioenergetics*, **2021**, 1862, 148382	4.6	2
82	Deactivation blocks proton pathways in the mitochondrial complex I. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	6
81	Fe-chitosan complexes for oxidative degradation of emerging contaminants in water: Structure, activity, and reaction mechanism. *Journal of Hazardous Materials*, **2021**, 408, 124662	12.8	6
80	The central role of the metal ion for photoactivity: Zn- Ni-Mabiq. *Chemical Science*, **2021**, 12, 7521-7532	9.4	7
79	Architecture of bacterial respiratory chains. *Nature Reviews Microbiology*, **2021**, 19, 319-330	22.2	23
78	Resolving Chemical Dynamics in Biological Energy Conversion: Long-Range Proton-Coupled Electron Transfer in Respiratory Complex I.. *Accounts of Chemical Research*, **2021**, 54, 4462-4473	24.3	2
77	Functional Water Wires Catalyze Long-Range Proton Pumping in the Mammalian Respiratory Complex I. *Journal of the American Chemical Society*, **2020**, 142, 21758-21766	16.4	12
76	Conformational dynamics modulate the catalytic activity of the molecular chaperone Hsp90. *Nature Communications*, **2020**, 11, 1410	17.4	24
75	A methylated lysine is a switch point for conformational communication in the chaperone Hsp90. *Nature Communications*, **2020**, 11, 1219	17.4	12
74	Exploring the catalytic cascade of cembranoid biosynthesis by combination of genetic engineering and molecular simulations. *Computational and Structural Biotechnology Journal*, **2020**, 18, 1819-1829	6.8	1
73	Water-Gated Proton Transfer Dynamics in Respiratory Complex I. *Journal of the American Chemical Society*, **2020**, 142, 13718-13728	16.4	18
72	Structural snapshots of the minimal PKS system responsible for octaketide biosynthesis. *Nature Chemistry*, **2020**, 12, 755-763	17.6	14
71	Redox-coupled proton pumping drives carbon concentration in the photosynthetic complex I. *Nature Communications*, **2020**, 11, 494	17.4	38
70	Ion Binding and Selectivity of the Na/H Antiporter MjNhaP1 from Experiment and Simulation. *Journal of Physical Chemistry B*, **2020**, 124, 336-344	3.4	1

69	Benchmarking the Performance of Time-Dependent Density Functional Theory Methods on Biochromophores. *Journal of Chemical Theory and Computation*, **2020**, 16, 587-600	6.4	32
68	Structure of inhibitor-bound mammalian complex I. *Nature Communications*, **2020**, 11, 5261	17.4	26
67	Reciprocal Coupling in Chemically Fueled Assembly: A Reaction Cycle Regulates Self-Assembly and Vice Versa. *Journal of the American Chemical Society*, **2020**, 142, 20837-20844	16.4	21
66	Dynamic Vesicles Formed By Dissipative Self-Assembly. *ChemSystemsChem*, **2020**, 2, e1900044	3.1	34
65	Dispersion forces drive water oxidation in molecular ruthenium catalysts.. *RSC Advances*, **2020**, 11, 425-432	3.7	2
64	Electric field modulated redox-driven protonation and hydration energetics in energy converting enzymes. *Chemical Communications*, **2019**, 55, 6078-6081	5.8	10
63	Molecular mechanism of polyketide shortening in anthraquinone biosynthesis of. *Chemical Science*, **2019**, 10, 6341-6349	9.4	9
62	How cardiolipin modulates the dynamics of respiratory complex I. *Science Advances*, **2019**, 5, eaav1850	14.3	37
61	Absorption shifts of diastereotopically ligated chlorophyll dimers of photosystem I. *Physical Chemistry Chemical Physics*, **2019**, 21, 6851-6858	3.6	12
60	Energetics and Dynamics of Proton-Coupled Electron Transfer in the NADH/FMN Site of Respiratory Complex I. *Journal of the American Chemical Society*, **2019**, 141, 5710-5719	16.4	19
59	Quantum Chemical and QM/MM Models in Biochemistry. *Methods in Molecular Biology*, **2019**, 2022, 75-104	1.4	3
58	Autophosphorylation activates c-Src kinase through global structural rearrangements. *Journal of Biological Chemistry*, **2019**, 294, 13186-13197	5.4	7
57	Redox- and Light-Driven Hydration Dynamics in Biological Energy Transduction **2019**, 53-81		
56	Site-specific ubiquitylation and SUMOylation using genetic-code expansion and sortase. *Nature Chemical Biology*, **2019**, 15, 276-284	11.7	55
55	Molecular dynamics and structural models of the cyanobacterial NDH-1 complex. *Biochimica Et Biophysica Acta - Bioenergetics*, **2019**, 1860, 201-208	4.6	7
54	The low spin - high spin equilibrium in the S-state of the water oxidizing enzyme. *Biochimica Et Biophysica Acta - Bioenergetics*, **2018**, 1859, 342-356	4.6	54
53	Long-range proton-coupled electron transfer in biological energy conversion: towards mechanistic understanding of respiratory complex I. *Journal of the Royal Society Interface*, **2018**, 15,	4.1	79
52	A switch point in the molecular chaperone Hsp90 responding to client interaction. *Nature Communications*, **2018**, 9, 1472	17.4	25

51	C-H Oxidation by a Diiron Complex with Facially Opposing Active Sites. *ChemistrySelect*, **2018**, 3, 1602-1608	2.8	3
50	Global collective motions in the mammalian and bacterial respiratory complex I. *Biochimica Et Biophysica Acta - Bioenergetics*, **2018**, 1859, 326-332	4.6	14
49	The protease GtgE from Salmonella exclusively targets inactive Rab GTPases. *Nature Communications*, **2018**, 9, 44	17.4	15
48	Catalytic mechanism and molecular engineering of quinolone biosynthesis in dioxygenase AsqJ. *Nature Communications*, **2018**, 9, 1168	17.4	20
47	Conformational Selection of Dimethylarginine Recognition by the Survival Motor Neuron Tudor Domain. *Angewandte Chemie*, **2018**, 130, 495-499	3.6	
46	Conformational Selection of Dimethylarginine Recognition by the Survival Motor Neuron Tudor Domain. *Angewandte Chemie - International Edition*, **2018**, 57, 486-490	16.4	1
45	Dewetting transitions coupled to K-channel activation in cytochrome oxidase. *Chemical Science*, **2018**, 9, 6703-6710	9.4	11
44	Redox-coupled quinone dynamics in the respiratory complex I. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, E8413-E8420	11.5	53
43	How inter-subunit contacts in the membrane domain of complex I affect proton transfer energetics. *Biochimica Et Biophysica Acta - Bioenergetics*, **2018**, 1859, 734-741	4.6	12
42	Energetics and dynamics of a light-driven sodium-pumping rhodopsin. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 7043-7048	11.5	52
41	Hsp90 dependence of a kinase is determined by its conformational landscape. *Scientific Reports*, **2017**, 7, 43996	4.9	19
40	To catalyze or not to catalyze: elucidation of the subtle differences between the hexameric capsules of pyrogallolarene and resorcinarene. *Chemical Science*, **2017**, 8, 1653-1657	9.4	39
39	Terminal Electron-Proton Transfer Dynamics in the Quinone Reduction of Respiratory Complex I. *Journal of the American Chemical Society*, **2017**, 139, 16282-16288	16.4	41
38	Symmetry-related proton transfer pathways in respiratory complex I. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, E6314-E6321	11.5	70
37	Correlating kinetic and structural data on ubiquinone binding and reduction by respiratory complex I. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 12737-12742	11.5	58
36	A Protonated Water Cluster as a Transient Proton-Loading Site in Cytochrome c Oxidase. *Angewandte Chemie - International Edition*, **2016**, 55, 11940-4	16.4	27
35	Oxidative Unfolding of the Rubredoxin Domain and the Natively Disordered N-terminal Region Regulate the Catalytic Activity of Mycobacterium tuberculosis Protein Kinase G. *Journal of Biological Chemistry*, **2016**, 291, 27062-27072	5.4	8
34	Redox-coupled substrate water reorganization in the active site of Photosystem II-The role of calcium in substrate water delivery. *Biochimica Et Biophysica Acta - Bioenergetics*, **2016**, 1857, 740-8	4.6	79

33	Tuning the Protein-Induced Absorption Shifts of Retinal in Engineered Rhodopsin Mimics. *Chemistry - A European Journal*, **2016**, 22, 8254-61	4.8	17
32	Conversion of light-energy into molecular strain in the photocycle of the photoactive yellow protein. *Physical Chemistry Chemical Physics*, **2016**, 18, 2802-9	3.6	15
31	Exploring the Light-Capturing Properties of Photosynthetic Chlorophyll Clusters Using Large-Scale Correlated Calculations. *Journal of Chemical Theory and Computation*, **2016**, 12, 2644-51	6.4	26
30	New perspectives on proton pumping in cellular respiration. *Chemical Reviews*, **2015**, 115, 2196-221	68.1	175
29	Protein-Induced Color Shift of Carotenoids in Crustacyanin. *Angewandte Chemie - International Edition*, **2015**, 54, 11564-6	16.4	42
28	Redox-induced activation of the proton pump in the respiratory complex I. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, 11571-6	11.5	86
27	Conformational processing of oncogenic v-Src kinase by the molecular chaperone Hsp90. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, E3189-98	11.5	62
26	Protein-induzierte Farbverschiebung von Carotenoiden in Crustacyanin. *Angewandte Chemie*, **2015**, 127, 11726-11729	3.6	7
25	Accessory NUMM (NDUFS6) subunit harbors a Zn-binding site and is essential for biogenesis of mitochondrial complex I. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, 5685-90	11.5	60
24	Linear energy relationships in ground state proton transfer and excited state proton-coupled electron transfer. *Journal of Physical Chemistry B*, **2015**, 119, 2611-9	3.4	20
23	Coupled-cluster studies of extensive green fluorescent protein models using the reduced virtual space approach. *Journal of Physical Chemistry B*, **2015**, 119, 2933-45	3.4	28
22	Contradictions in X-ray structures of intermediates in the photocycle of photoactive yellow protein. *Nature Chemistry*, **2014**, 6, 258-9	17.6	25
21	Spectral tuning of rhodopsin and visual cone pigments. *Journal of the American Chemical Society*, **2014**, 136, 2723-6	16.4	40
20	Electrostatics, hydration, and proton transfer dynamics in the membrane domain of respiratory complex I. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 6988-93	11.5	76
19	Electrostatic spectral tuning mechanism of the green fluorescent protein. *Physical Chemistry Chemical Physics*, **2013**, 15, 4491-5	3.6	36
18	Dynamic water networks in cytochrome cbb3 oxidase. *Biochimica Et Biophysica Acta - Bioenergetics*, **2012**, 1817, 726-34	4.6	16
17	The effect of protein environment on photoexcitation properties of retinal. *Journal of Physical Chemistry B*, **2012**, 116, 2249-58	3.4	39
16	Reduction of the virtual space for coupled-cluster excitation energies of large molecules and embedded systems. *Journal of Chemical Physics*, **2011**, 134, 214114	3.9	52

15	The identity of the transient proton loading site of the proton-pumping mechanism of cytochrome c oxidase. *Biochimica Et Biophysica Acta - Bioenergetics*, **2011**, 1807, 80-4	4.6	67
14	A combined quantum chemical and crystallographic study on the oxidized binuclear center of cytochrome c oxidase. *Biochimica Et Biophysica Acta - Bioenergetics*, **2011**, 1807, 769-78	4.6	30
13	Stabilization of the peroxy intermediate in the oxygen splitting reaction of cytochrome cbb(3). *Biochimica Et Biophysica Acta - Bioenergetics*, **2011**, 1807, 813-8	4.6	14
12	Aromatic pathways in conjugated rings connected by single bonds. *International Journal of Quantum Chemistry*, **2011**, 111, 848-857	2.1	16
11	Energetics and dynamics of proton transfer reactions along short water wires. *Physical Chemistry Chemical Physics*, **2011**, 13, 13207-15	3.6	43
10	Energetics of direct and water-mediated proton-coupled electron transfer. *Journal of the American Chemical Society*, **2011**, 133, 19040-3	16.4	27
9	Benchmarking the Approximate Second-Order Coupled-Cluster Method on Biochromophores. *Journal of Chemical Theory and Computation*, **2011**, 7, 2473-84	6.4	39
8	Proton-coupled electron transfer in cytochrome oxidase. *Chemical Reviews*, **2010**, 110, 7062-81	68.1	414
7	Interheme electron tunneling in cytochrome c oxidase. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 21470-5	11.5	20
6	Redox-coupled proton transfer in the active site of cytochrome cbb3. *Biochimica Et Biophysica Acta - Bioenergetics*, **2010**, 1797, 1512-20	4.6	13
5	The chemistry of the CuB site in cytochrome c oxidase and the importance of its unique His-Tyr bond. *Biochimica Et Biophysica Acta - Bioenergetics*, **2009**, 1787, 221-33	4.6	41
4	Mechanism and energetics by which glutamic acid 242 prevents leaks in cytochrome c oxidase. *Biochimica Et Biophysica Acta - Bioenergetics*, **2009**, 1787, 1205-14	4.6	46
3	Prevention of leak in the proton pump of cytochrome c oxidase. *Biochimica Et Biophysica Acta - Bioenergetics*, **2008**, 1777, 890-2	4.6	21
2	Glutamic acid 242 is a valve in the proton pump of cytochrome c oxidase. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 6255-9	11.5	114
1	Charge parameterization of the metal centers in cytochrome c oxidase. *Journal of Computational Chemistry*, **2008**, 29, 753-67	3.5	45