Curriculum Vitae of Prof. Dr. Ville R. I. Kaila

CONTACT AND PERSONAL INFORMATION

Jan, 2021

Name:	Ville Rolf Ilmari Kaila
Address (work):	Department of Biochemistry and Biophysics Stockholm University
Date of birth:	December 6, 1983 (age 37)
Civil status:	Married, two children (born 2013, 2019)
Country of citizenship:	Finland
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EDUCATION

2007-2009	**Ph.D.** in Theoretical Biochemistry, University of Helsinki, Finland. Ph.D. Thesis: "Theoretical Studies on Coupled Electron and Proton Transfer in Cytochrome *c* Oxidase". Grade: *excellent* (April/2009)
2003-2006	**M.Sc.** in Biochemistry, University of Helsinki, Finland. Extended minors in Physical Chemistry, Physics and Theoretical Physics.
1994-2004	Sibelius Academy, Finland. Training for a solo violin career.

LEAVE OF ABSENCE

2009-2010	Compulsory military service (Finland), 13 months.

RESEARCH AND PROFESSIONAL EXPERIENCE

2019-present	**Full Professor** of Biochemistry, Department of Biochemistry and Biophysics, Stockholm University, Sweden.
2018-2019	**Professor (W3)** of Computational Biocatalysis, Department of Chemistry, Technical University Munich (TUM), Germany.
2013-2018	**Tenure-track Professor (W2 to W3)** of Computational Biocatalysis, Department of Chemistry, Technical University Munich (TUM), Germany.
2013	Offer for **Assistant Professor (W1)** at the Department of Chemistry and Biochemistry, Free University Berlin, Germany (declined).
2011	**Docent (Adjunct Professor)** of Physical Biochemistry, University of Helsinki.
2010-2013	**Post-doctoral researcher**, Laboratory of Chemical Physics (LCP), NIDDK, National Institutes of Health (NIH). Mentor: Gerhard Hummer
2010-2012	**Long-Term Postdoctoral Fellow**, European Molecular Biology Organization.
2010	**Short-term post-doctoral researcher**, University of Helsinki, Finland. Mentor: Prof. Dage Sundholm
2006-2010	**Temporary Lecturer**, Department of Biology and Department of Chemistry, University of Helsinki, Finland.
2005-2009	**Researcher**, Helsinki Bioenergetics Group, University of Helsinki, Finland. Mentor: Prof. Mårten Wikström
2008	**Visiting scholar** in the research group of Prof. Peter Taylor, University of Warwick, UK.
2005	**Research assistant** in NMR-laboratory, University of Helsinki, Finland.
2004	**Research assistant** in Helsinki Bioenergetics Group, University of Helsinki, Finland.

PUBLICATIONS SUMMARY AND INVITED TALKS (summary)

***ca*. 90 peer-reviewed articles** (see publications list below), 3500 citations in total, *h*-index 33 (Google scholar), including multiple publications in *e.g*. *PNAS (11)*, *Nature Chemistry (2)*, *Nature Comm (7)*, *Nature Chem Biol* (1), *Science Adv* (1), *Angew Chemie* (4), *Chem Rev* (2), *Chem Science* (2)*,* and *JACS* (7); **> 60** invited/plenary talks during 2014-present.

SUPERVISED RESEARCH

10 post-docs (4 now at PI/senior scientist positions), 16 PhD students (7 completed; 9 in progress), >20 research internships/BSc/MSc-theses. Lectured/developed *ca*. 20 courses during 2013-present.

HONORS, AWARDS, AND GRANTS (selected)

2020	**Research Grant** from Swedish Research Council (VR), 4.9 Mio SEK.
2020	**Research Grant** from Swedish Cancerfoundation 1.6 Mio SEK.
2019	**Wallenberg Academy Fellow**.
2019	**Recognition award:** Sven & Ebba-Christina Hagberg foundation
2019	**Wallenberg foundation project**, 38 Mio SEK, Team: Högbom-Ädelroth-Brzezinski-Kaila, "*The obligate respiratory supercomplex – augmented biological energy conversion"*.
2019	**Recognition award:** Ruth & Nils-Erik Stenbäck's foundation.
2018	**Recognition award:** Hans Fischer Memorial Award.
2018	**Excellence in teaching nomination, TU Munich**.
2018-2019	**Research funding** from Center of Integrated Protein Science Munich, 35,000 EUR.
2016	**European Research Council (ERC),** Starting Grant, "bioPCET", 1.5 Mio EUR for five years.
2015-2020	Several **research grants** from German Research Foundation (DFG), in total *ca.* 1.3 Mio EUR including TRR235 and SFB1035; Molecular Mechanism of Energy Conversion in Respiratory Complex I.
2015	**Recognition award:** The Grand Prize, Oskar Öflund's foundation.
2015-2016	**German Researcher exchange grant**, "Computational Studies of Electronically Excited States of Biochromophores", 23 500 EUR.
2014-2015	**Research grant** from Jane and Aatos Erkko Foundation: "Mechanisms of Biomimetic Water Splitting", 89 000 EUR.
2010-2012	**Long-Term Postdoctoral Fellow**, European Molecular Biology Organization (EMBO).
2010	**Recognition award** from Ruth & Nils-Erik Stenbäck's foundation, the Finnish Science Foundation.
2009	**The Alfthan's prize** of the Finnish Chemical Society for best doctoral thesis of 2009 in Chemistry in Finland.
2007-2009	**Ph.D. fellowship** from Helsinki Graduate School of Biotechnology and Molecular Biology, University of Helsinki, Finland.
2006	**Research Award** from Finnish Cultural Foundation.

PROFESSIONAL EXPERIENCE (selected)

2020-present	Elected Foreign Member of the Finnish Society of Sciences and Letters.
2014-present	Served in **>40 PhD committees** as examiner/opponent/chair.
2018-present	**Editorial board member** of the J. Royal Society of Interface.
2017-2018	**Second chairman** of Munich Chemical Society (MChG).
2010-present	**Reviewer** for Angew Chemie, BBA, Biochemistry, Biol Chem, Biophys J, ChemPhysChem, eLife, FEBS Lett, Int J Quant Chem, JACS, J Comput Chem, J Phys Chem, J Phys Chem Lett, NSMB, NComms, Nature, Nature Chem PCCP, PLOS journals, PNAS, Science, Sci Rep. etc.
2014-present	**Grant reviewer** for Humboldt Found., DAAD, DFG, ISF, NWO, ERC. Supercomputing Centers: Jülich, Irish, SuperMUC, Psi-K network.

10 Selected Publications of Prof. Ville R. I. Kaila

(See full publications list below)

1. Mühlbauer ME, Saura P, Nuber F, Di Luca A, Friedrich T, **Kaila VRI** (2020) Water-gated proton transfer dynamics in respiratory complex I. ***J Am Chem Soc*** 142: 13718-13728.

2. Schuller JM, Saura P, Thiemann J, Schuller S, Gamiz-Hernandez AP, Kurisu G, Nowaczyk MM, **Kaila VRI** (2020) Redox-Coupled Proton Pumping Drives Carbon Concentration in the Photosynthetic Complex I, ***Nature Comms*** 11, 494: 1-7.

3. Jussupow A, Di Luca A, **Kaila VRI** (2019) How cardiolipin modulates the activity of complex I. ***Science Adv*** 5, eaav1850.

4. Warnau J, Sharma V, Gamiz-Hernandez AP, Di Luca A, Haapanen O, Vattulainen I, Wikström M, Hummer G, **Kaila VRI** (2018) Redox-Coupled Quinone Dynamics in the Respiratory Complex I. ***PNAS*** 115: E8413-E8420.

5. Mader SL, Bräuer A, Groll M, **Kaila VRI** (2018) Catalytic mechanism and molecular engineering of quinolone biosynthesis in dioxygenase AsqJ. ***Nature Comm*** 9, 1168:1-8.

6. Gamiz-Hernandez AP, Jussupow A, Johansson MP, **Kaila VRI** (2017) Terminal Electron-Proton Transfer Dynamics coupled to Quinone reduction in Respiratory Complex I. ***JACS*** 139:16282-16288.

7. Suomivuori C-M, Gamiz-Hernandez AP, Sundholm D, **Kaila VRI** (2017) Energetics and dynamics of a light-driven sodium-pumping rhodopsin. ***PNAS*** 114:7043-7048. Cover issue.

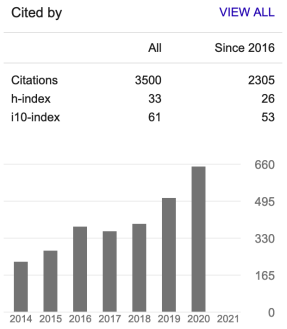
8. Di Luca A, Gamiz-Hernandez AP, **Kaila VRI** (2017) Symmetry related proton transfer pathways in respiratory Complex I. ***PNAS*** 114:E6314-E6321.

9. Sharma V, Belevich G, Gamiz-Hernandez AP, Róg T, Vattulainen I, Wikström M, Hummer G, **Kaila VRI** (2015) Redox-Induced Activation of the Proton Pump in the Respiratory Complex I. ***PNAS*** 112:11571-11576.

10. **Kaila VRI**, Wikström M, Hummer G (2014) Electrostatics, Hydration, and Proton Transfer Dynamics in the Membrane Domain of Respiratory Complex I. ***PNAS*** 111:6988-6993.

PUBLICATIONS of Prof. Ville R. I. Kaila (updated Jan 2021)

N=94 incl. 5 in review; 3500 citations, *h*-index 33 (Google scholar)
* corresponding author



94. Röpke M, Saura P, Riepl D, Pöverlein M, **Kaila VRI*** (2020) Functional water-wires catalyze long-range proton pumping in the mammalian respiratory complex I. **J Am Chem Soc** 142:21758-21766.

93. Bridges HR, Fedor JG, Blaza JN, Di Luca A, Jussupow A, Jarman OD, Wright J, Agip ANA, Gamiz-Hernandez AP, Roessler MM, **Kaila VRI***, Hirst J (2020) Structure of inhibitor-bound mammalian complex I, **Nature Comms,** 5261: 11, 1–11.

92. Kriebisch BAK, Jussupow A, Bergmann AM, Kohler F, Dietz H, **Kaila VRI**, Boekhoven J (2020) Reciprocal Coupling in Chemically Fueled Assembly: A Reaction Cycle Regulates Self-Assembly and Vice Versa. **J Am Chem Soc** 142(49):20837-20844.

91. Johansson MP, Niederegger L; Rauhalahti M; Hess CR; **Kaila VRI*** (2021) Dispersion-Forces Drive Water Oxidation in Molecular Ruthenium Catalysts. **RSC Advances** 11, 425-432.

90. Kaila VRI*, Wikström M (2021) Architecture of Bacterial Respiratory Chains. **Nature Rev Microbiol** (in press) doi: 10.1038/s41579-020-00486-4

89. Mühlbauer ME, Saura P, Nuber F, Di Luca A, Friedrich T, **Kaila VRI*** (2020) Water-gated proton transfer dynamics in respiratory complex I. **J Am Chem Soc** 142, 13718-13728.

88. Schuller JM, Saura P, Thiemann J, Schuller S, Gamiz-Hernandez AP, Kurisu G, Nowaczyk MM, **Kaila VRI*** (2020) Redox-Coupled Proton Pumping Drives Carbon Concentration in the Photosynthetic Complex I, **Nature Comms** 11, 494: 1-7.

87. Mader SL, Lopez A, Lawatscheck J, Luo Q, Rutz DA, Gamiz-Hernandez AP, Sattler M, Buchner J, **Kaila VRI*** (2020) Conformational dynamics modulate the catalytic activity of the molecular chaperone Hsp90. **Nature Comms** 11: 11410; 1-12.

86. Rehn A, Lawatscheck J, Mader SL, Luo Q, Blank B, Richter K, **Kaila VRI,** Buchner, J (2020) A methylated lysine is a switch point for conformational communication in the chaperone Hsp90. **Nature Comms** 11: 1219; 1-14.

85. Bräuer A, Zhou Q, Grammbitter GLC, Schmalhofer M, **Kaila VRI**, Bode HB, Groll M (2020) Structural Snapshots of the Minimal PKS System Responsible for Octaketide Biosynthesis. **Nature Chemistry** 12(8):755-763.

84. Wild R, Di Luca A, Bisha I, **Kaila VRI*** (2020) Ligand-dependent structural dynamics drives conformational switching in the human serotonin transporter (in review).

83. Röpke M, Riepl D, Di Luca A, Saura P, Mühlbauer M, Jussupow A, Gamiz-Hernandez AP, **Kaila VRI*** (2020) Deactivation blocks proton pathways in the mitochondrial complex I (in review).

82. Di Luca A, **Kaila VRI*** (2020) Molecular strain in the active/deactive-transition modulates domain coupling in respiratory complex I (in review).

81. Baumgart M, Röpke M, Mühlbauer ME, Asami S, Mader S, Fredriksson K, Groll M, Gamiz-Hernandez AP, **Kaila VRI*** (2020) Design of Buried Charged Networks in Artificial Proteins (in review).

80. Farinelli G, Di Luca A, **Kaila VRI**, MacLachlan MJ, Tiraferri A (2020), Fe-chitosan complexes for oxidative degradation of emerging contaminants in water: Structure, activity, and reaction mechanism. **J. Hazard Mater.** 124662. doi.org/10.1016/j.jhazmat.2020.124662

79. Wanzke C, Jussupow A, Kohler F, Dietz H, **Kaila VRI,** Boekhoven J (2020) Dynamic vesicles formed by dissipative self-assembly, **ChemSystemsChem** *2,* e1900044.

77. Shao Y, Mei Y, Sundholm D, **Kaila VRI**[*] (2020) Benchmarking the performance of time-dependent density functional theory methods on biochromophores. **J Chem Theor Comput** 16: 587-600.

76. Lauenstein R; Mader S; Derondeau H; Block M; Römer A; Jandl C; Riedle E; **Kaila VRI,** Hauer J; Thyrhaug E; Hess CR (2020). The central role of the metal ion in photocatalysis: Zn- vs. Ni-Mabiq. (in review).

75. Warnau J, Wöhlert D, Okazaki K, Yildiz O, Gámiz-Hernández AP, **Kaila VRI**[*], Kühlbrandt W, Hummer G (2020) Ion Binding and Selectivity of the Na^+/H^+ Antiporter MjNhaP1. **J. Phys Chem B** 124: 336-344.

74. Kaila VRI[*] (2019) Molekularen Mechanismen der biologischen Energieumwandlung. **Nachr Chem** 67.

73. Saura P, **Kaila VRI**[*] (2019) Energetics and Dynamics of NADH-Driven Proton-Coupled Electron Transfer in Respiratory Complex I. **J Am Chem Soc** 41: 5710-5719.

72. Jussupow A, Di Luca A, **Kaila VRI**[*] (2019) How cardiolipin modulates the activity of complex I. **Science Adv** 5, eaav1850.

71. Schrepfer P, Ugur I, Klumpe S., Metterlein M, Loll B, **Kaila VRI**[*], Brück T (2020) Exploring the catalytic cascade of cembranoid biosynthesis by combination of genetic engineering and molecular simulations. **Comput Struct Biotechnol J** 18:1819-1829.

70. Suomivuori CM, Fliegl H, Starikov EB, Balaban TS, **Kaila VRI**, and Sundholm D (2019) Absorption Shifts of Diastereotopically Ligated Chlorophyll Dimers of Photosystem I. ***Phys Chem Chem Phys*** 21, 6851-6858.

69. Kaila VRI[*] (2019) Redox- and light-driven hydration dynamics (2019) in Oxygen Production and Reduction in Artificial and Natural Systems, *Eds*. *J. Barber, A. Ruban, P. Nixon*.

68. Jagtap PKA, Asami S, Sippel C, **Kaila VRI**, Hausch F, Sattler M (2019). Selective inhibitors of FKBP51 employ conformational selection of dynamic invisible states. ***Angew Chemie Intl. Ed***. 58:9429-9433.

67. Saura P, Frey D, Gamiz-Hernandez AP, **Kaila VRI**[*] (2019) Electric Field Modulated Redox-Driven Protonation and Hydration Energetics in Energy Converting Enzymes. ***Chem Comm*** 55(43):6078-6081.

66. Zhou Q, Bräuer A, Adihou H, Schmalhofer M, Saura P, **Kaila VRI**, Groll M, Bode H (2019) Molecular mechanism of polyketide shortening in anthraquinone biosynthesis of *Photorhabdus luminescens.* ***Chem Science*** 10:6341-6349.

65. Boczek E, Luo Q, Dehling M, Röpke M, Mader S, Seidl A, **Kaila VRI**[*], Buchner J (2019) Auto-phosphorylation activates c-Src kinase through global structural rearrangements. ***J Biol Chem*** 294:13186-13197.

64. Fottner M, Brunner A-D, Bittl V, Horn-Ghetko D, Jussupow A, **Kaila VRI**, Bremm A, Lang K (2019) Site-specific ubiquitylation and SUMOylation using genetic code expansion and sortase-mediated transpeptidation. ***Nature Chem Biol*** 5:276-284.

63. Saura P, **Kaila VRI**[*] (2018) Structure and dynamics of the cyanobacterial NDH-1 complex. **Biochim Biophys Acta - Bioenerg** 1860:201-208.

62. Warnau J, Sharma V, Gamiz-Hernandez AP, Di Luca A, Haapanen O, Vattulainen I, Wikström M, Hummer G, **Kaila VRI**[*] (2018) Redox-Coupled Quinone Dynamics in the Respiratory Complex I. **Proc Natl Acad Sci USA** 115: E8413-E8420.

61. Mader SL, Bräuer A, Groll M, **Kaila VRI**[*] (2018) Catalytic mechanism and molecular engineering of quinolone biosynthesis in dioxygenase AsqJ. **Nature Comm** 9, 1168: 1-8.

60. Supekar S, **Kaila VRI**[*] (2018) Dewetting transitions coupled to K-channel activation in cytochrome *c* oxidase. **Chem Science** 9: 6703-6710.

59. Di Luca A, Mühlbauer M, Saura P, **Kaila VRI*** (2018) How inter-subunit contacts in the membrane domain of complex I affect proton transfer energetics **Biochim Biophys Acta - Bioenerg** 1859: 734-741.

58. Kaila VRI[*] (2018) Long-Range Proton-Coupled Electron Transfer in Biological Energy Conversion: Towards Mechanistic Understanding of Respiratory Complex I. **J. R. Soc. Interfaces** 15: 20170916.

57. Saura P, Röpke M, Gamiz-Hernandez AP, **Kaila VRI**[*] (2019) Quantum Chemical and QM/MM Models in Biochemistry. **Methods in Mol Biol** 2022:75-104.

56. Lindsay S, Mader SL, **Kaila VRI*,** Hess CR (2018) C-H Oxidation by a Diiron Complex with Facially Opposing Active Sites. **ChemistrySelect** 3(5).

55. Boussac A, Ugur I, Marion A, Sugiura M, **Kaila VRI**, Rutherford AW (2018) The low spin - high spin equilibrium in the S2-state of the water oxidizing enzyme. **Biochim Biophys Acta - Bioenerg** 1859: 342-356.

54. Di Luca, **Kaila VRI**[*] (2018) Global Collective Motions in the Mammalian and Bacterial Respiratory Complex I. **Biochim Biophys Acta - Bioenerg** 1859: 326-332.

53. Fedor J, Di Luca A, **Kaila VRI**, Hirst J (2017) Correlating kinetic and structural data on ubiquinone binding and reduction by respiratory complex I. **Proc Natl Acad Sci USA** 114: 12737-12742.

52. Rutz DA, Luo Q, Freiburger L, Madl T, **Kaila VRI**, Sattler M, Buchner J (2018) A switch point in the molecular chaperone Hsp90 responding to client interaction. **Nature Comm** 9: 1472.

51. Kaila VRI[*] (2018) Multi-scale Molecular Simulations on Respiratory Complex I. in Chemical Biology No. 5, "Mechanisms of Primary Energy Transduction in Biology", *Ed*. Mårten Wikström, **The Royal Society of Chemistry** 2018 doi:10.1039/9781788010405-00081.

50. Wachtel R, Bräuning B, Mader SL, Ecker F, **Kaila VRI**, Groll M, Itzen A (2018) The protease GtgE from Salmonella exclusively targets inactive Rab-proteins. **Nature Comm** 9: 44.

49. Gamiz-Hernandez AP, Jussupow A, Johansson MP, **Kaila VRI**[*] (2017) Terminal Electron-Proton Transfer Dynamics coupled to Quinone reduction in Respiratory Complex I**. J Am Chem Soc** 139: 16282-16288.

48. Suomivuori C-M, Gamiz-Hernandez AP, Sundholm D, **Kaila VRI**[*] (2017) Energetics and dynamics of a light-driven sodium-pumping rhodopsin. **Proc Natl Acad Sci USA** 114: 7043-7048. Cover issue.

47. Supekar S, Papageorgiou AC, Gemmecker G, Peltzer R, Johansson MP, Tripsianes K, Sattler M, **Kaila VRI**[*] (2018) Conformational Selection of Dimethylarginine Recognition by the SMN Tudor Domain. **Angew Chemie Intl Ed** 57: 486-490.

46. Di Luca A, Gamiz-Hernandez AP, **Kaila VRI**[*] (2017) Symmetry related proton transfer pathways in respiratory Complex I. **Proc Natl Acad Sci USA** 114: E6314-E6321.

45. Luo Q, Boczek EE, Buchner J, **Kaila VRI**[*] (2017) Conformational activation and Hsp90-dependence of c-Src and its oncogenic mutants. **Sci Rep** 7: 43996.

44. Suomivuori C-M, Winter N.O.C., Hättig C, Sundholm D, **Kaila VRI**[*] (2016) Exploring the Light-Capturing Properties of Photosynthetic Chlorophyll Clusters Using Large-Scale Correlated Calculations. **J Chem Theory Comput** 12: 2644-2651.

43. Wittwer M, Luo Q, **Kaila VRI**, Dames S (2016) Oxidative Unfolding of the Rubredoxin Domain and the Natively Disordered N-terminal Region Regulate the Catalytic Activity of M. tuberculosis Protein Kinase G. **J Mol Biol** 291: 27062-27072.

42. Gamiz-Hernandez AP, **Kaila VRI**[*] (2016) Conversion of light-energy into molecular strain in the photocycle of the photoactive yellow protein. **Phys Chem Chem Phys** 18: 2802-2809.

41. Zhang Q, Catti L, **Kaila VRI**, Tiefenbacher K (2016) To Catalyze or not to Catalyze: Elucidation of the Subtle Differences between the Hexameric Capsules of Pyrogallolarene and Resorcinarene. **Chem Sci** 8: 1653-1657.

40. Suomivuori CM, Lang L, Sundholm D, Gamiz-Hernandez AP, **Kaila VRI**[*] (2016) Tuning the protein-induced absorption shifts of retinal in engineered rhodopsin mimics. **Chem – Eur J**. 22: 8254-8861.

39. Supekar S, Gamiz-Hernandez AP, **Kaila VRI**[*] (2016) A Protonated Water Cluster as a Transient Proton Loading Site in Cytochrome c Oxidase. **Angew Chemie Intl Ed** 55: 11940-11944.

38. Ugur I, Rutherford AW, **Kaila VRI**[*] (2016) Redox-coupled substrate water reorganization in the active site of Photosystem II. **Biochim Biophys Acta – Bioenerg** 1857: 740-748.

37. Sharma V, Belevich G, Gamiz-Hernandez AP, Róg T, Vattulainen I, Wikström M, Hummer G, **Kaila VRI**[*] (2015) Redox-Induced Activation of the Proton Pump in the Respiratory Complex I. **Proc Natl Acad Sci USA** 112:11571-11576.

36. Gamiz-Hernandez AP, Neycheva IA, Send R, Sundholm D, **Kaila VRI**[*] (2015) Protein-Induced Color Shift of Carotenoids in β-Crustacyanin. **Angew Chemie Intl Ed** 54:11564-11566.

35. Boczek EE, Reefschläger LG, Dehling M, Struller T, Häusler E, Seidl A, **Kaila VRI**, Buchner J (2015) Conformational processing of oncogenic v-Src kinase by Hsp90. **Proc Natl Acad Sci USA** 112: E3189-3198.

34. Kmita K, Wirth C, Warnau J, Guerrero-Castillo S, Hunte C, Hummer G, **Kaila VRI**, Zwicker K, Brandt U, Zickermann V. (2015) Accessory NUMM (NDUFS6) subunit harbors a Zn-binding site and is essential for biogenesis of mitochondrial complex I. **Proc Natl Acad Sci USA** 112: 5685-5690.

33. Wikström M, Sharma V, **Kaila VRI**, Hosler J, Hummer G (2015) New perspectives on proton pumping in cellular respiration. **Chem Rev** 115: 2196-2221.

32. Send R, Suomivuori CM, **Kaila VRI**[*], Sundholm D (2015) Coupled-Cluster Studies of Extensive Green Fluorescent Protein Models using the Reduced Virtual Space Approach**. J Phys Chem B** 119: 2933-2945.

31. Gamiz-Hernandez AP, Magomedov A, Hummer G, **Kaila VRI**[*] (2014) Linear energy relationships in ground state proton transfer and excited state proton-coupled electron transfer **J Phys Chem B** 119: 2611-2619.

30. Kaila VRI[*], Wikström M, Hummer G (2014) Electrostatics, Hydration, and Proton Transfer Dynamics in the Membrane Domain of Respiratory Complex I. **Proc Natl Acad Sci USA** 111: 6988-6993.

29. Kaila VRI, Schotte F, Hyun S-C, Hummer G, Anfinrud PA (2014) Reconciling contradictions in time-resolved x-ray structures of early intermediates in the photocycle of photoactive yellow protein. **Nature Chem** 6: 258-259.

28. Zhou X, Sundholm D, Wesolowski A, **Kaila VRI**[*] (2014) Spectral Tuning of Rhodopsin and Visual Cone Pigments. **J Am Chem Soc** 136: 2723-2726.

27. Kaila VRI[*], Send R, Sundholm D (2013) Electrostatic Spectral Tuning Mechanism of the Green Fluorescent Protein. **Phys Chem Chem Phys** 15: 4491-4495.

26. Johansson MP, **Kaila VRI**[*], Sundholm D (2013) *Ab initio*, density functional theory, and semi-empirical calculations. **Methods in Mol Biol** 924: 3-27.

25. Schotte F, Hyun S-C, **Kaila VRI**, Kamikubo H, Dashdorja N, Henry E, Graber T, Henning R, Wulff M, Hummer G, Kataoka M, Anfinrud PA (2012) Picosecond Photobiology: Watching a Signaling Protein Function in Real Time via Time-resolved Laue Crystallography. **Proc Natl Acad Sci USA** 109: 19256-19261.

24. Kaila VRI[*], Send R, Sundholm D (2012) The effect of the protein environment on primary photoexcitation events of retinal. **J Phys Chem B** 116: 2249-2258.

23. Sharma V, Wikström M, **Kaila VRI**[*] (2012) Dynamic water networks in cytochrome cbb_3. **Biochim Biophys Acta – Bioenerg** 1817: 726-734.

22. Kaila VRI[*], Hummer G (2011) Energetics of direct and water-mediated proton-coupled electron transfer. **J Am Chem Soc** 133: 19040-19043.

21. Kaila VRI[*], Hummer G (2011) Energetics and dynamics of proton transfer reactions along short water wires. **Phys Chem Chem Phys** 13: 13207-13215.

20. Send R, **Kaila VRI**, Sundholm D (2011) Benchmarking the Approximate Second-Order Coupled-Cluster Method on Biochromophores. **J Chem Theory Comput** 7: 2473-2484.

19. Send R, **Kaila VRI**, Sundholm D (2011) Reduction of the virtual space for coupled-cluster excitation energies of large molecules and embedded systems. **J Chem Phys** 134: 214114.

18. Sharma V, Wikström M, **Kaila VRI**[*] (2011) Stabilization of the peroxy intermediate in the oxygen splitting reaction of cytchrome cbb_3. **Biochim Biophys Acta** 1807: 813-818.

17. Kaila VRI[*], Oksanen E, Goldman A, Verkhovsky MI, Sundholm D, Wikström M (2011) A Combined Quantum Chemical and Crystallographic Study on the Oxidized Binuclear Center of Cytochrome *c* Oxidase. **Biochim Biophys Acta – Bioenerg** 1807: 769-778.

16. Fliegl H, Lehtonen O, Sundholm D, **Kaila VRI**[*] (2011) Hydrogen-bond strengths by magnetically induced currents. **Phys Chem Chem Phys** 13: 434-437.

15. Kaila VRI[*], Sharma V, Wikström M (2011) The identity of the transient proton loading site of the proton-pumping mechanism of cytochrome *c* oxidase. **Biochim Biophys Acta – Bioenerg** 1807: 80-84.

14. Taubert S, **Kaila VRI**, Sundholm D (2011) Aromatic pathways in conjugated rings connected by single bonds. **Int J Quantum Chem** 111: 848-857.

13. Kaila VRI, Verkhovsky MI, Wikström M (2010) Proton-coupled electron transfer in cytochrome oxidase. **Chem Rev** 110: 7062-7081.

12. Kaila VRI[*], Johansson MP, Sundholm D, Wikström M (2010) Interheme electron tunneling in cytochrome *c* oxidase. **Proc Natl Acad Sci USA** 107: 21470-21475.

11. Sharma V, Wikström M, **Kaila VRI**[*] (2010) Redox-coupled proton transfer in the active site of cytochrome cbb_3. **Biochim Biophys Acta – Bioenerg** 1797: 1512-1520.

10. Kaila VRI[*], Verkhovsky MI, Hummer G, Wikström M (2009) Mechanism and energetics by which glutamic acid 242 prevents leaks in cytochrome *c* oxidase. **Biochim Biophys Acta – Bioenerg** 1787: 1205-1214.

9. Kaila VRI, Johansson MP, Sundholm D, Laakkonen L, Wikström M (2009) The chemistry of the CuB site in cytochrome *c* oxidase and the importance of its unique His Tyr bond. **Biochim Biophys Acta – Bioenerg** 1787: 221-233.

8. Sharma V, **Kaila VRI**, Annila A (2009) Protein folding as an evolutionary process. **Physica A** 388: 851-862.

7. Kaila VRI, Annila A (2008) Natural selection for least action. **Proc Roy Soc A** 464: 3055-3070.

6. Kaila VRI, Verkhovsky MI, Hummer G, Wikström M (2008) Prevention of leak in the proton pump of cytochrome *c* oxidase. **Biophys Biochim Acta – Bioenerg** 1777: 890-892.

5. Kaila VRI, Verkhovsky MI, Hummer G, Wikström M (2008) Glutamic acid 242 is a valve in the proton pump of cytochrome *c* oxidase. **Proc Natl Acad Sci USA** 105: 6255-6259.

4. Johansson MP, **Kaila VRI**, Laakkonen L (2008) Charge parameterization of the metal centers in cytochrome *c* oxidase. **J Comput Chem** 29: 753-767.

3. Tuukkanen A[*a*], **Kaila VRI**[*a*]**,** Laakkonen L, Hummer G, Wikström M (2008) Dynamics of the glutamic acid 242 side chain in cytochrome *c* oxidase. **Biochim Biophys Acta – Bioenerg** 1767: 1102-1106 ([*a*]shared first authorship).

2. Kaila VRI (2009), "Theoretical Studies on Coupled Electron and Proton Transfer in Cytochrome Oxidase". ISBN 978-952-10- 5263-7, ISSN 1795-7079, Yliopistopaino, Helsinki.

1. Kaila VRI (2006) "Beräkningskemiska studier av proton-translokeringsmekanismen i cytokrom *c* oxidas", MSc thesis.