

List of Publications
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- [1] Klaus Schulten and Martin Karplus. On the origin of a low-lying forbidden transition in polyenes and related molecules. *Chem. Phys. Lett.*, 14:305–309, 1972.
- [2] Robert R. Birge, Klaus Schulten, and Martin Karplus. Possible influence of a low-lying “covalent” excited state on the absorption spectrum and photoisomerization of 11-cis retinal. *Chem. Phys. Lett.*, 31:451–454, 1975.
- [3] Klaus Schulten and Roy G. Gordon. Exact recursive evaluation of $3j$ - and $6j$ -coefficients for quantum-mechanical coupling of angular momenta. *J. Math. Phys.*, 16:1961–1970, 1975.
- [4] Klaus Schulten and Roy G. Gordon. Semiclassical approximation to $3j$ - and $6j$ -coefficients for quantum-mechanical coupling of angular momenta. *J. Math. Phys.*, 16:1971–1988, 1975.
- [5] Klaus Schulten, I. Ohmine, and Martin Karplus. Correlation effects in the spectra of polyenes. *J. Chem. Phys.*, 64:4422–4441, 1976.
- [6] Klaus Schulten and Roy G. Gordon. Quantum theory of angular momentum coupling in reactive collisions. *J. Chem. Phys.*, 64:2918–2938, 1976.
- [7] Klaus Schulten and Roy G. Gordon. Recursive evaluation of $3j$ - and $6j$ -coefficients. *Comput. Phys. Commun.*, 11:269–278, 1976.
- [8] Klaus Schulten, H. Staerk, Albert Weller, Hans-Joachim Werner, and B. Nickel. Magnetic field dependence of the geminate recombination of radical ion pairs in polar solvents. *Z. Phys. Chem.*, NF101:371–390, 1976.
- [9] Klaus Schulten. Quantum mechanical propensity rules for the transfer of angular momentum in three-atom reactions. *Ber. Bunsenges. Phys. Chem.*, 81:166–168, 1977.
- [10] Zhan Schulten and Klaus Schulten. The generation, diffusion, spin motion, and recombination of radical pairs in solution in the nanosecond time domain. *J. Chem. Phys.*, 66:4616–4634, 1977.
- [11] Hans-Joachim Werner, Zhan Schulten, and Klaus Schulten. Theory of the magnetic field modulated geminate recombination of radical ion pairs in polar solvents: Application to the pyrene-N,N-dimethylaniline system. *J. Chem. Phys.*, 67:646–663, 1977.
- [12] I. Ohmine, Martin Karplus, and Klaus Schulten. Renormalized configuration interaction method for electron correlation in the excited states of polyenes. *J. Chem. Phys.*, 68:2298–2318, 1978.
- [13] Klaus Schulten and Paul Tavan. A mechanism for the light-driven proton pump of *Halobacterium halobium*. *Nature*, 272:85–86, 1978.
- [14] Hans-Joachim Werner, Klaus Schulten, and Albert Weller. Electron transfer and spin exchange contributing to the magnetic field dependence of the primary photochemical reaction of bacterial photosynthesis. *Biochim. Biophys. Acta*, 502:255–268, 1978.
- [15] Paul Tavan and Klaus Schulten. The ‘phantom’ photochemical singlet state of stilbene and its diphenylpolyene relative. *Chem. Phys. Lett.*, 56:200–204, 1978.
- [16] Klaus Schulten and Peter G. Wolynes. Semiclassical description of electron spin motion in radicals including the effect of electron hopping. *J. Chem. Phys.*, 68:3292–3297, 1978.

- [17] Klaus Schulten and Albert Weller. Exploring fast electron transfer processes by magnetic fields. *Bio-phys. J.*, 24:295–305, 1978.
- [18] Klaus Schulten. An isomerization model for the photocycle of bacteriorhodopsin. In S. R. Caplan and M. Ginzburg, editors, *Energetics and Structure of Halophilic Organisms*, pp. 331–334. Elsevier, 1978.
- [19] Klaus Schulten, Charles E. Swenberg, and Albert Weller. A biomagnetic sensory mechanism based on magnetic field modulated coherent electron spin motion. *Z. Phys. Chem.*, NF111:1–5, 1978.
- [20] G. Orlandi and Klaus Schulten. Coupling of stereochemistry and proton donor–acceptor properties of a Schiff base: A model of a light-driven proton pump. *Chem. Phys. Lett.*, 64:370–374, 1979.
- [21] Paul Tavan and Klaus Schulten. The $2^1A_g - 1^1B_u$ energy gap in the polyenes: An extended configuration interaction study. *J. Chem. Phys.*, 70:5407–5413, 1979.
- [22] Paul Tavan and Klaus Schulten. Correlation effects in the spectra of polyacenes. *J. Chem. Phys.*, 70:5414–5421, 1979.
- [23] Klaus Schulten and Irving R. Epstein. Recombination of radical pairs in high magnetic fields: A path integral–Monte Carlo treatment. *J. Chem. Phys.*, 71:309–316, 1979.
- [24] Ernst-Walter Knapp and Klaus Schulten. Magnetic field effect on the hyperfine-induced electron spin motion in radicals undergoing diamagnetic–paramagnetic exchange. *J. Chem. Phys.*, 71:1878–1883, 1979.
- [25] Ernst-Walter Knapp, Klaus Schulten, and Zan Schulten. Proton conduction in linear hydrogen-bonded systems. *Chem. Phys.*, 46:215–229, 1980.
- [26] Klaus Schulten, Zan Schulten, and Attila Szabo. Reactions governed by a binomial redistribution process. The Ehrenfest urn problem. *Physica*, 100A:599–614, 1980.
- [27] Paul Tavan and Klaus Schulten. An efficient approach to CI: General matrix element formulas for spin-coupled particle-hole excitations. *J. Chem. Phys.*, 72:3547–3576, 1980.
- [28] Attila Szabo, Klaus Schulten, and Zan Schulten. First passage time approach to diffusion controlled reactions. *J. Chem. Phys.*, 72:4350–4357, 1980.
- [29] Uri Dinur, Barry Honig, and Klaus Schulten. On the nature of excited electronic states in cyanine dyes: Implications for visual pigment spectra. *Chem. Phys. Lett.*, 72:493–497, 1980.
- [30] Klaus Schulten, Uri Dinur, and Barry Honig. The spectra of carbonium ions, cyanine dyes, and protonated Schiff base polyenes. *J. Chem. Phys.*, 73:3927–3935, 1980.
- [31] Klaus Schulten, Zan Schulten, and Attila Szabo. Dynamics of reactions involving diffusive barrier crossing. *J. Chem. Phys.*, 74:4426–4432, 1981.
- [32] Reiner Peters, Axel Brünger, and Klaus Schulten. Continuous fluorescence microphotolysis: A sensitive method for study of diffusion processes in single cells. *Proc. Natl. Acad. Sci. USA*, 78:962–966, 1981.
- [33] Gene Lamm and Klaus Schulten. Extended Brownian dynamics approach to diffusion-controlled processes. *J. Chem. Phys.*, 75:365–371, 1981.
- [34] Klaus Schulten. Magnetic field effects in chemistry and biology. In J. Treusch, editor, *Festkörperprobleme*, volume 22, pp. 61–83. Vieweg, Braunschweig, 1982.
- [35] Bruce S. Hudson, Bryan E. Kohler, and Klaus Schulten. Linear polyene electronic structure and potential surfaces. In Edward C. Lim, editor, *Excited States*, volume 6, pp. 1–95. Academic Press, New York, 1982.

- [36] Gene Lamm and Klaus Schulten. Extended Brownian dynamics: II. Reactive, nonlinear diffusion. *J. Chem. Phys.*, 78:2713–2734, 1983.
- [37] Walter Nadler and Klaus Schulten. Generalized moment expansion for the Mössbauer spectrum of Brownian particles. *Phys. Rev. Lett.*, 51:1712–1715, 1983.
- [38] Klaus Schulten. Ensemble averaged spin pair dynamics of doublet and triplet molecules. In P. Reineker, H. Haken, and H. C. Wolf, editors, *Organic Molecular Aggregates*, pp. 76–87. Springer, 1983.
- [39] Axel Brünger, Zan Schulten, and Klaus Schulten. A network thermodynamic investigation of stationary and non-stationary proton transport through proteins. *Z. Phys. Chem.*, NF136:1–63, 1983.
- [40] Klaus Schulten. Ensemble averaged spin pair dynamics of doublet and triplet molecules. *J. Chem. Phys.*, 80:3668–3679, 1984.
- [41] Klaus Schulten, Axel Brünger, Walter Nadler, and Zan Schulten. Generalized moment description of Brownian dynamics in biological systems. In E. Frehland, editor, *Synergetics — From Microscopic to Macroscopic Order*, pp. 80–89. Springer, 1984.
- [42] Klaus Schulten, Zan Schulten, and Paul Tavan. An isomerization model for the pump cycle of bacteriorhodopsin. In L. Bolis, E. J. M. Helmreich, and H. Passow, editors, *Information and Energy Transduction in Biological Membranes*, pp. 113–131. Allan R. Liss, Inc., New York, 1984.
- [43] Walter Nadler and Klaus Schulten. Theory of Mössbauer spectra of proteins fluctuating between conformational substates. *Proc. Natl. Acad. Sci. USA*, 81:5719–5723, 1984.
- [44] Paul Tavan and Klaus Schulten. The effect of protonation on the thermal isomerization of stilbazolium betaines. *Chem. Phys. Lett.*, 110:191–195, 1984.
- [45] Klaus Schulten and Albert Weller. Magnetfeldeffekte in Chemie und Biologie. *Die Umschau*, 25/26:779–783, 1984.
- [46] Paul Tavan, Klaus Schulten, and Dieter Oesterhelt. The effect of protonation and electrical interactions on the stereochemistry of retinal Schiff bases. *Biophys. J.*, 47:415–430, 1985.
- [47] Zan Schulten and Klaus Schulten. Model for the resistance of the proton channel formed by the proteolipid of ATPase. *Eur. Biophys. J.*, 11:149–155, 1985.
- [48] Paul Tavan, Klaus Schulten, Wolfgang Gärtner, and Dieter Oesterhelt. Substituents at the C₁₃ position of retinal and their influence on the function of bacteriorhodopsin. *Biophys. J.*, 47:349–356, 1985.
- [49] Axel Brünger, Reiner Peters, and Klaus Schulten. Continuous fluorescence microphotolysis to observe lateral diffusion in membranes: Theoretical methods and applications. *J. Chem. Phys.*, 82:2147–2160, 1985.
- [50] Klaus Schulten. The effect of intramolecular paramagnetic–diamagnetic exchange on the magnetic field effect of radical pair recombination. *J. Chem. Phys.*, 82:1312–1316, 1985.
- [51] Walter Nadler and Klaus Schulten. Generalized moment expansion for Brownian relaxation processes. *J. Chem. Phys.*, 82:151–160, 1985.
- [52] Walter Nadler, Paul Tavan, and Klaus Schulten. A model for the lateral diffusion of ‘stiff’ chains in a lipid bilayer. *Eur. Biophys. J.*, 12:25–31, 1985.
- [53] Herbert Treutlein and Klaus Schulten. Noise induced limit cycles of the Bonhoeffer–van der Pol model of neural pulses. *Ber. Bunsenges. Phys. Chem.*, 89:710–718, 1985.
- [54] Walter Nadler and Klaus Schulten. Mean relaxation time approximation for dynamical correlation functions in stochastic systems near instabilities. *Z. Physik B*, 59:53–61, 1985.

- [55] M. Scholz, Klaus Schulten, and Reiner Peters. Single-cell flux measurement by continuous fluorescence microphotolysis. *Eur. Biophys. J.*, 13:37–44, 1985.
- [56] Robert Bittl, Herbert Treutlein, and Klaus Schulten. Electron conduction along aliphatic chains. In M. Michel-Beyerle, editor, *Antennas and Reaction Centers of Photosynthetic Bacteria — Structure, Interaction and Dynamics*, pp. 264–276. Springer, 1985.
- [57] Joachim Buhmann, Helge Ritter, and Klaus Schulten. Neuro-kybernetik und künstliche Intelligenz. *Computerwoche*, 25, 1985.
- [58] Zan Schulten and Klaus Schulten. Proton conduction through proteins: An overview of theoretical principles and applications. *Meth. Enzym.*, 127:419–438, 1986.
- [59] Herbert Treutlein and Klaus Schulten. Noise-induced neural impulses. *Eur. Biophys. J.*, 13:355–365, 1986.
- [60] Walter Nadler and Klaus Schulten. Generalized moment expansion for observables of stochastic processes in dimensions $d > 1$: Application to Mössbauer spectra of proteins. *J. Chem. Phys.*, 84:4015–4025, 1986.
- [61] Klaus Schulten and Robert Bittl. Probing the dynamics of a polymer with paramagnetic end groups by magnetic fields. *J. Chem. Phys.*, 84:5155–5161, 1986.
- [62] Helge Ritter and Klaus Schulten. On the stationary state of Kohonen’s self-organizing sensory mapping. *Biol. Cyber.*, 54:99–106, 1986.
- [63] Klaus Schulten. Continuous fluorescence microphotolysis by a $\sin^2 kx$ grating. *Chem. Phys. Lett.*, 124:230–236, 1986.
- [64] Paul Tavan and Klaus Schulten. Evidence for a 13,14-cis cycle in bacteriorhodopsin. *Biophys. J.*, 50:81–89, 1986.
- [65] Joachim Buhmann and Klaus Schulten. Associative recognition and storage in a model network of physiological neurons. *Biol. Cyber.*, 54:319–335, 1986.
- [66] Joachim Buhmann and Klaus Schulten. A physiological neural network as an autoassociative memory. In E. Bienenstock, F. Fogelman, and G. Weisbuch, editors, *Disordered Systems and Biological Organization*, pp. 273–279. Springer, 1986.
- [67] Dieter Oesterhelt, P. Hegemann, Paul Tavan, and Klaus Schulten. Trans-cis isomerization of retinal and a mechanism for ion translocation in halorhodopsin. *Eur. Biophys. J.*, 14:123–129, 1986.
- [68] Robert Bittl and Klaus Schulten. Study of polymer dynamics by magnetic field dependent biradical reactions. In G. Maret, N. Boccarda, and J. Kiepenheuer, editors, *Biophysical Effects of Steady Magnetic Fields*, volume 11 of *Proceedings in Physics*, pp. 90–98. Springer, Berlin, 1986.
- [69] Klaus Schulten. Magnetic field effects on radical pair processes in chemistry and biology. In J. H. Bernhard, editor, *Biological Effects of Static and Extremely Low Frequency Magnetic Fields*, pp. 133–140. MMV Medizin Verlag, Munich, 1986.
- [70] Klaus Schulten and Andreas Windemuth. Model for a physiological magnetic compass. In G. Maret, N. Boccarda, and J. Kiepenheuer, editors, *Biophysical Effects of Steady Magnetic Fields*, volume 11 of *Proceedings in Physics*, pp. 99–106. Springer, Berlin, 1986.
- [71] Joachim Buhmann and Klaus Schulten. Influence of noise on the behaviour of an autoassociative neural network. In J. S. Denker, editor, *Neural Networks for Computing*, pp. 71–76. American Institute of Physics Publication, Conference Proceedings 151, 1986.

- [72] Helge Ritter and Klaus Schulten. Topology conserving mappings for learning motor tasks. In J. S. Denker, editor, *Neural networks for computing*, pp. 376–380. American Institute of Physics publication, conference proceedings 151, 1986.
- [73] Robert Divko and Klaus Schulten. Stochastic spin models for pattern recognition. In J. S. Denker, editor, *Neural Networks for Computing*, pp. 129–134. American Institute of Physics Publication, Conference Proceedings 151, 1986.
- [74] Paul Tavan and Klaus Schulten. The low-lying electronic excitations in long polyenes: A PPP–MRD–CI study. *J. Chem. Phys.*, 85:6602–6609, 1986.
- [75] Helge Ritter and Klaus Schulten. Planning a dynamic trajectory via path finding in discretized phase space. In *Parallel Processing: Logic, Organization, and Technology*, volume 253 of *Lecture Notes in Computer Science*, pp. 29–39. Springer, 1987.
- [76] Joachim Buhmann, Robert Divko, Helge Ritter, and Klaus Schulten. Physicists explore human and artificial intelligence. In *Structure and Dynamics of Nucleic Acids, Proteins and Membranes*, pp. 301–328. Plenum Press, 1986.
- [77] Joachim Buhmann and Klaus Schulten. Influence of noise on the function of a “physiological” neural network. *Biol. Cyber.*, 56:313–327, 1987.
- [78] Joachim Buhmann and Klaus Schulten. Noise-driven temporal association in neural networks. *Europhys. Lett.*, 4:1205–1209, 1987.
- [79] Paul Tavan and Klaus Schulten. Electronic excitations in finite and infinite polyenes. *Phys. Rev. B*, 36:4337–4358, 1987.
- [80] Kim Sharp, Richard Fine, Klaus Schulten, and Barry Honig. Brownian dynamics simulation of diffusion to irregular bodies. *Phys. Chem.*, 91:3624–3631, 1987.
- [81] Klaus Schulten. Ordnung aus Chaos, Vernunft aus Zufall — Physik biologischer und digitaler Informationsverarbeitung. In B.-O. Küppers, editor, *Ordnung aus dem Chaos*, pp. 243–268. Piper Verlag, Munich, 1987.
- [82] Walter Nadler, Axel Brünger, Klaus Schulten, and Martin Karplus. Molecular and stochastic dynamics of proteins. *Proc. Natl. Acad. Sci. USA*, 84:7933–7937, 1987.
- [83] Joachim Buhmann, Robert Divko, Helge Ritter, and Klaus Schulten. Physik und Gehirn — Wie dynamische Modelle von Nervennetzen natürliche Intelligenz erklären. *MC-Computermagazin*, 9:108–120, 1987.
- [84] Joseph Eccles, Barry Honig, and Klaus Schulten. Spectroscopic determinants in the reaction center of *Rhodospseudomonas viridis*. *Biophys. J.*, 53:137–144, 1988.
- [85] Helge Ritter and Klaus Schulten. Extending Kohonen’s self-organizing mapping algorithm to learn ballistic movements. In R. Eckmiller and Ch. von der Malsburg, editors, *Neural Computers*, volume 41 of *NATO Sci. Ser. F*, pp. 393–406. Springer-Verlag, 1988.
- [86] Joachim Buhmann and Klaus Schulten. Storing sequences of biased patterns in neural networks with stochastic dynamics. In R. Eckmiller and Ch. von der Malsburg, editors, *Neural Computers*, Computer and Systems Sciences, pp. 231–242. Springer, 1988.
- [87] Herbert Treutlein, Andreas Windemuth, and Klaus Schulten. “Molecular Design” — Simulation und Graphik von Biomolekülen. *MC-Computermagazin*, 1:46–57, 1988.
- [88] Paul Tavan and Klaus Schulten. Quasiparticle excitations in polyenes and polyacetylene. In A. J. Heeger, J. Orenstein, and D. Ulrich, editors, *Nonlinear Optical Properties of Polymers*, volume 109 of *Symposium Proceedings*, pp. 163–170. Materials Research Society, Pittsburgh, 1988.

- [89] Hans-Ulrich Bauer, Klaus Schulten, and Walter Nadler. Generalized moment expansion of dynamic correlation functions in finite Ising systems. *Phys. Rev. B*, 38:445–458, 1988.
- [90] Herbert Treutlein, Klaus Schulten, J. Deisenhofer, H. Michel, Axel Brünger, and Martin Karplus. Molecular dynamics simulation of the primary processes in the photosynthetic reaction center of *Rhodospseudomonas viridis*. In J. Breton and A. Verméglio, editors, *The Photosynthetic Bacterial Reaction Center: Structure and Dynamics*, volume 149 of *NATO Sci. Ser. A*, pp. 139–150. Plenum, New York, 1988.
- [91] Herbert Treutlein, Klaus Schulten, Christoph Niedermeier, J. Deisenhofer, H. Michel, and D. Devault. Electrostatic control of electron transfer in the photosynthetic reaction center of *Rhodospseudomonas viridis*. In J. Breton and A. Verméglio, editors, *The Photosynthetic Bacterial Reaction Center: Structure and Dynamics*, volume 149 of *NATO Sci. Ser. A*, pp. 369–377. Plenum, New York, 1988.
- [92] Robert Bittl and Klaus Schulten. Length dependence of the magnetic field modulated triplet yield of photogenerated biradicals. *Chem. Phys. Lett.*, 146:58–62, 1988.
- [93] Klaus Boehncke, Christoph Köhler, Georg Meyer-Berg, and Klaus Schulten. Eine Computersimulation künstlicher Wesen — Experimente in einer Welt synthetischer Psychologie. *MC-Computermagazin*, 7:34–48, 1988.
- [94] Robert Bittl and Klaus Schulten. A static ensemble approximation for stochastically modulated quantum systems. *J. Chem. Phys.*, 90:1794–1803, 1989.
- [95] Helge Ritter and Klaus Schulten. Convergence properties of Kohonen’s topology conserving maps: Fluctuations, stability and dimension selection. *Biol. Cyber.*, 60:59–71, 1988.
- [96] Walter Nadler and Klaus Schulten. Mean relaxation time approximation for dynamical correlation functions in stochastic systems near instabilities: II. The single mode laser. *Z. Physik*, 72:535–543, 1988.
- [97] Joachim Buhmann, Robert Divko, and Klaus Schulten. Associative memory with high information content. *Phys. Rev. A*, 39:2689–2692, 1989.
- [98] Helge Ritter and Klaus Schulten. Kohonen’s self-organizing maps: Exploring their computational capabilities. In *IEEE International Conference on Neural Networks, San Diego, California, July 24–27, 1988*, volume 1, pp. 109–116, New York, 1988. The Institute of Electrical and Electronics Engineers.
- [99] Joachim Buhmann and Klaus Schulten. Invariant pattern recognition by means of fast synaptic plasticity. In *IEEE International Conference on Neural Networks, San Diego, California, July 24–27, 1988*, volume 1, pp. 125–132, New York, 1988. The Institute of Electrical and Electronics Engineers.
- [100] Helmut Grubmüller, Helmut Heller, and Klaus Schulten. Eine Cray für 100.000 DM. *MC-Computermagazin*, 11:48–64, 1988.
- [101] Herbert Treutlein, Christoph Niedermeier, Klaus Schulten, J. Deisenhofer, H. Michel, Axel Brünger, and Martin Karplus. Molecular dynamics simulation of the primary processes in the Photosynthetic reaction center of *Rhodospseudomonas viridis*. In A. Pullman et al., editors, *Transport Through Membranes: Carriers, Channels and Pumps*, pp. 513–525. Kluwer Academic Publishers, Dordrecht, 1988.
- [102] Michael F. Grossjean, Paul Tavan, and Klaus Schulten. Can normal mode analysis reveal the geometry of the L₅₅₀ chromophore of bacteriorhodopsin? *Eur. Biophys. J.*, 16:341–349, 1989.
- [103] Helge Ritter, Thomas Martinetz, and Klaus Schulten. Wie neuronale Netwerke Roboter steuern können. *MC-Computermagazin*, 2:48–61, 1989.
- [104] Helge Ritter, Thomas Martinetz, and Klaus Schulten. Topology-conserving maps for learning visuo-motor-coordination. *Neur. Netw.*, 2:159–168, 1989.

- [105] Jeanne Rubner and Klaus Schulten. A regularized approach to color constancy. *Biol. Cyber.*, 61:29–36, 1989.
- [106] Helge Ritter, Thomas Martinetz, and Klaus Schulten. Topology-conserving maps for motor control. In L. Personnaz and G. Dreyfus, editors, *Neural Networks: From Models to Applications, N'EURO '88*, pp. 579–591. EZIDET, Paris, 1989.
- [107] Joachim Buhmann, Robert Divko, and Klaus Schulten. On sparsely coded associative memories. In L. Personnaz and G. Dreyfus, editors, *Neural Networks: From Models to Applications, N'EURO '88*, pp. 360–371. EZIDET, Paris, 1989.
- [108] Thomas Martinetz, Helge Ritter, and Klaus Schulten. 3D-neural-net for learning visuomotor-coordination of a robot arm. In *Proceedings of the International Joint Conference on Neural Networks, Washington*, volume 2, pp. 351–356, San Diego, 1989. The Institute of Electrical and Electronics Engineers.
- [109] Thomas Martinetz, Helge Ritter, and Klaus Schulten. Kohonen's self-organizing map for modeling the formation of the auditory cortex of a bat. In R. Pfeifer, Z. Schreter, F. Fogelman-Soulié, and L. Steels, editors, *Connectionism in Perspective*, pp. 403–412. North-Holland, Amsterdam, 1989.
- [110] Helge Ritter, Thomas Martinetz, and Klaus Schulten. *Textbook: Neuronale Netze: Eine Einführung in die Neuroinformatik selbstorganisierender Abbildungen*. Addison-Wesley, Bonn, first edition, 1990.
- [111] Helmut Heller, Helmut Grubmüller, and Klaus Schulten. Molecular dynamics simulation on a parallel computer. *Mol. Sim.*, 5:133–165, 1990.
- [112] Markus van Almsick and Klaus Schulten. Mathematica: Mathematik auf Mikrocomputern. *MC-Computermagazin*, 11:42–59, 1989.
- [113] Robert Bittl and Klaus Schulten. Biradical spin dynamics with distance-dependent exchange interaction and electron transfer efficiency. *Chem. Phys. Lett.*, 173:387–392, 1990.
- [114] Thomas Martinetz, Helge Ritter, and Klaus Schulten. Three-dimensional neural net for learning visuomotor coordination of a robot arm. *IEEE Trans. Neur. Netw.*, 1:131–136, 1990.
- [115] Jeanne Rubner and Klaus Schulten. Development of feature detectors by self-organization: A network model. *Biol. Cyber.*, 62:193–199, 1990.
- [116] Klaus Obermayer, Helge Ritter, and Klaus Schulten. Large-scale simulation of a self-organizing neural network: Formation of a somatotopic map. In R. Eckmiller, G. Hartmann, and G. Hauske, editors, *Parallel Processing in Neural Systems and Computers*, pp. 71–74. Elsevier, Amsterdam, 1990.
- [117] Thomas Martinetz, Helge Ritter, and Klaus Schulten. Learning of visuo motor-coordination of a robot arm with redundant degrees of freedom. In R. Eckmiller, G. Hartmann, and G. Hauske, editors, *Parallel Processing in Neural Systems and Computers*, pp. 431–434. Elsevier, Amsterdam, 1990.
- [118] Robert Divko and Klaus Schulten. Hierarchical spin model for stereo interpretation using phase sensitive detectors. In R. Eckmiller, G. Hartmann, and G. Hauske, editors, *Parallel Processing in Neural Systems and Computers*, pp. 335–338. Elsevier, Amsterdam, 1990.
- [119] Jeanne Rubner, Klaus Schulten, and Paul Tavan. A self-organizing network for complete feature extraction. In R. Eckmiller, G. Hartmann, and G. Hauske, editors, *Parallel Processing in Neural Systems and Computers*, pp. 365–368. Elsevier, Amsterdam, 1990.
- [120] Christian Kurrer and Klaus Schulten. Propagation of chemical waves in discrete excitable media: Anisotropic and isotropic wave fronts. In A. V. Holden, M. Markus, and H. G. Othmer, editors, *Nonlinear Wave Processes in Excitable Media*, volume 244 of *NATO Sci. Ser. B*, pp. 489–500. Plenum Press, New York, 1991.

- [121] Robert Bittl, Klaus Schulten, and Nick Turro. Micellar radical pair decay. *J. Chem. Phys.*, 93:8260–8269, 1990.
- [122] Helge Ritter, Thomas Martinetz, and Klaus Schulten. *Textbook: Neuronale Netze: Eine Einführung in die Neuroinformatik selbstorganisierender Abbildungen*. Addison-Wesley, Bonn, second enlarged edition, 1990.
- [123] Herbert Treutlein, Klaus Schulten, Axel Brünger, Martin Karplus, J. Deisenhofer, and H. Michel. Chromophore-protein interactions and the function of the photosynthetic reaction center: A molecular dynamics study. *Proc. Natl. Acad. Sci. USA*, 89:75–79, 1992.
- [124] Michael F. Grossjean, Paul Tavan, and Klaus Schulten. Quantum chemical vibrational analysis of the chromophore of bacteriorhodopsin. *J. Phys. Chem.*, 94:8059–8069, 1990.
- [125] Wolfgang R. Bauer and Klaus Schulten. Theory of contrast agents in magnetic resonance imaging: Coupling of spin relaxation and transport. *Magn. Res. Med.*, 26:16–39, 1992.
- [126] M. K. Grossjean, Michael F. Grossjean, Klaus Schulten, and Paul Tavan. Semistochastic approach to many electron systems. *J. Chem. Phys.*, 97:1865–1875, 1992.
- [127] Andreas Windemuth and Klaus Schulten. Molecular dynamics simulation on the Connection Machine. *Mol. Sim.*, 5:353–361, 1991.
- [128] Markus Tesch and Klaus Schulten. A simulated cooling process for proteins. *Chem. Phys. Lett.*, 169:97–102, 1990.
- [129] Daniel Barsky, Benno Pütz, Klaus Schulten, and Richard L. Magin. Theory of paramagnetic contrast agents in liposome systems. *Magn. Res. Med.*, 24:1–13, 1992.
- [130] Jörg A. Walter, Helge Ritter, and Klaus Schulten. Non-linear prediction with self-organizing maps. In *International Joint Conference on Neural Networks, San Diego, California*, volume 1, pp. 589–594. The Institute of Electrical and Electronics Engineers, New York, 1990.
- [131] Klaus Obermayer, Helge Ritter, and Klaus Schulten. A neural network model for the formation of topographic maps in the CNS: Development of receptive fields. In *International Joint Conference on Neural Networks, San Diego, California*, volume 2, pp. 423–429. The Institute of Electrical and Electronics Engineers, New York, 1990.
- [132] Thomas Martinetz and Klaus Schulten. Hierarchical neural net for learning control of a robot’s arm and gripper. In *International Joint Conference on Neural Networks, San Diego, California*, volume 2, pp. 747–752. The Institute of Electrical and Electronics Engineers, New York, 1990.
- [133] Klaus Obermayer, Helge Ritter, and Klaus Schulten. Large-scale simulations of self-organizing neural networks on parallel computers: Application to biological modelling. *Parall. Comp.*, 14:381–404, 1990.
- [134] Marco Nonella and Klaus Schulten. Molecular dynamics simulation of electron transfer in proteins: Theory and application to $Q_A \rightarrow Q_B$ transfer in the photosynthetic reaction center. *J. Phys. Chem.*, 95:2059–2067, 1991.
- [135] Andreas Windemuth and Klaus Schulten. Stochastic dynamics simulation for macromolecules. Beckman Institute Technical Report TB-91-19, University of Illinois, 1991.
- [136] Helge Ritter, Klaus Obermayer, Klaus Schulten, and Jeanne Rubner. Self-organizing maps and adaptive filters. In J. Leo van Hemmen, Eytan Domany, and Klaus Schulten, editors, *Models of Neural Networks, Physics of Neural Networks*, pp. 281–306. Springer-Verlag, New York, 1991.
- [137] Christian Kurrer and Klaus Schulten. Effect of noise and perturbations on limit cycle systems. *Physica D*, 50:311–320, 1991.

- [138] Klaus Obermayer, Helge Ritter, and Klaus Schulten. A principle for the formation of the spatial structure of cortical feature maps. *Proc. Natl. Acad. Sci. USA*, 87:8345–8349, 1990.
- [139] Klaus Boehncke, Helmut Heller, Helmut Grubmüller, and Klaus Schulten. Molecular dynamics simulations on a systolic ring of transputers. In Alan S. Wagner, editor, *NATUG 3: Transputer Research and Applications 3*, pp. 83–94, Amsterdam, 1990. North American Transputer Users Group, IOS Press.
- [140] Klaus Obermayer, Helmut Heller, Helge Ritter, and Klaus Schulten. Simulation of self-organizing neural nets: A comparison between a transputer ring and a Connection Machine CM-2. In Alan S. Wagner, editor, *NATUG 3: Transputer Research and Applications 3*, pp. 95–106, Amsterdam, 1990. North American Transputer Users Group, IOS Press.
- [141] Helmut Grubmüller, Helmut Heller, Andreas Windemuth, and Klaus Schulten. Generalized Verlet algorithm for efficient molecular dynamics simulations with long-range interactions. *Mol. Sim.*, 6:121–142, 1991.
- [142] Christoph Niedermeier and Klaus Schulten. Molecular dynamics simulations in heterogenous dielectrica and Debye-Hückel media: Application to the protein bovine pancreatic trypsin inhibitor. *Mol. Sim.*, 8:361–387, 1992.
- [143] Klaus Boehncke, Marco Nonella, Klaus Schulten, and Andrew H.-J. Wang. Molecular dynamics investigation of the interaction between DNA and dystamycin. *Biochemistry*, 30:5465–5475, 1991.
- [144] Christian Kurrer, Benno Nieswand, and Klaus Schulten. A model for synchronous activity in the visual cortex. In A. Babloyantz, editor, *Self-Organization, Emergent Properties, and Learning*, volume 260 of *NATO Sci. Ser. B*, pp. 81–95. Plenum Press, New York, 1991.
- [145] Klaus Obermayer, Helge Ritter, and Klaus Schulten. A model for the development of the spatial structure of retinotopic maps and orientation columns. *IEICE Trans. Fund. Electr. Comm. Comp. Sci.*, E75-A:537–545, 1992. Reprinted in *The Principles of Organization in Organisms — Santa Fe Institute Studies in the Sciences of Complexity, Vol. XII*. A. Baskin and J. Mittlethal, Eds. (Addison Wesley, 1991).
- [146] Klaus Schulten and Markus Tesch. Coupling of protein motion to electron transfer: Molecular dynamics and stochastic quantum mechanics study of photosynthetic reaction centers. *Chem. Phys.*, 158:421–446, 1991.
- [147] Benno Pütz, Daniel Barsky, and Klaus Schulten. Edge enhancement by diffusion in microscopic magnetic resonance imaging. *J. Magn. Reson.*, 97:27–53, 1992.
- [148] Thomas Martinetz and Klaus Schulten. A neural network for robot control: Cooperation between neural units as a requirement for learning. *Comp. & Elect. Engr.*, 19:315–332, 1993.
- [149] Thomas M. Martinetz, Stanislav G. Berkovich, and Klaus Schulten. “Neural gas” for vector quantization and its application to time-series prediction. *IEEE Trans. Neur. Netw.*, 4:558–569, 1993.
- [150] Thomas Martinetz and Klaus Schulten. A “neural gas” network learns topologies. In Teuvo Kohonen, Kai Mäkisara, Olli Simula, and Jari Kangas, editors, *Artificial Neural Networks*, pp. 397–402. Elsevier, Amsterdam, 1991.
- [151] Klaus Obermayer, Gary G. Blasdel, and Klaus Schulten. A neural network model for the formation and for the spatial structure of retinotopic maps, orientation- and ocular dominance columns. In Teuvo Kohonen, Kai Mäkisara, Olli Simula, and Jari Kangas, editors, *Artificial Neural Networks*, pp. 505–511. Elsevier, Amsterdam, 1991.
- [152] Edgar Erwin, Klaus Obermayer, and Klaus Schulten. Convergence properties of self-organizing maps. In Teuvo Kohonen, Kai Mäkisara, Olli Simula, and Jari Kangas, editors, *Artificial Neural Networks*, pp. 409–414. Elsevier, Amsterdam, 1991.

- [153] Jörg A. Walter, Thomas Martinetz, and Klaus Schulten. Industrial robot learns visuo-motor coordination by means of “neural gas” network. In Teuvo Kohonen, Kai Mäkisara, Olli Simula, and Jari Kangas, editors, *Artificial Neural Networks*, pp. 357–364. Elsevier, Amsterdam, 1991.
- [154] Christian Kurrer, Benno Nieswand, and Klaus Schulten. Dynamics of synchronous neural activity in the visual cortex. In Teuvo Kohonen, Kai Mäkisara, Olli Simula, and Jari Kangas, editors, *Artificial Neural Networks*, pp. 133–138. Elsevier, Amsterdam, 1991.
- [155] Klaus Obermayer, Helge Ritter, and Klaus Schulten. Development and spatial structure of cortical feature maps: A model study. In D. Touretzky and R. Lippman, editors, *Advances in Neural Information Processing Systems 3*, pp. 11–17. Morgan Kaufmann, San Mateo CA, 1991.
- [156] Marco Nonella, Andreas Windemuth, and Klaus Schulten. Structure of bacteriorhodopsin and *in situ* isomerization of retinal: A molecular dynamics study. *J. Photochem. Photobiol.*, 54:937–948, 1991.
- [157] Mark A. Shifman, Andreas Windemuth, Klaus Schulten, and Perry L. Miller. Molecular dynamics simulation on a network of workstations using a machine-independent parallel programming language. *Comp. Biomed. Res.*, 25:168–180, 1992.
- [158] Edgar Erwin, Klaus Obermayer, and Klaus Schulten. Formation of dimension-reducing somatotopic maps. In Samir I. Sayegh, editor, *Proceedings of the Fourth Conference on Neural Networks and Parallel Distributed Processing*, pp. 115–126. Indiana University at Fort Wayne, 1992.
- [159] Helge Ritter, Thomas Martinetz, and Klaus Schulten. *Textbook: Neural Computation and Self-Organizing Maps: An Introduction*. Addison-Wesley, New York, revised English edition, 1992.
- [160] Stanislav G. Berkovitch, Philippe Dalger, Ted Hesselroth, Thomas Martinetz, Benoît Noël, Jörg A. Walter, and Klaus Schulten. Vector quantization algorithm for time series prediction and visuo-motor control of robots. In W. Brauer and D. Hernandez, editors, *Verteilte Künstliche Intelligenz und kooperatives Arbeiten*, volume 291 of *Informatikfachberichte*, pp. 443–447. Springer, Berlin, 1991.
- [161] Benno Pütz, Daniel Barsky, and Klaus Schulten. Edge enhancement by diffusion: Microscopic magnetic resonance imaging of an ultra-thin glass capillary. *Chem. Phys. Lett.*, 183:391–396, 1991.
- [162] Wolfgang R. Bauer and Klaus Schulten. Nuclear spin dynamics ($I=1/2$) under the influence of random perturbation fields in the “strong collision” approximation. *Ber. Bunsenges. Phys. Chem.*, 96:721–727, 1992.
- [163] Edgar Erwin, Klaus Obermayer, and Klaus Schulten. Self-organizing maps: Ordering, convergence properties and energy functions. *Biol. Cyber.*, 67:47–55, 1992.
- [164] Edgar Erwin, Klaus Obermayer, and Klaus Schulten. Self-organizing maps: Stationary states, metastability and convergence rate. *Biol. Cyber.*, 67:35–45, 1992.
- [165] Klaus Schulten. Computational biology on massively parallel machines. In *Parallel Computation — Proceedings of the First International ACPC Conference, Salzburg, Austria*, pp. 391–400, New York, 1992. Springer.
- [166] Dong Xu and Klaus Schulten. Coupling of protein motion to electron transfer in a photosynthetic reaction center: Investigating the low temperature behaviour in the framework of the spin-boson model. *Chem. Phys.*, 182:91–117, 1994.
- [167] Klaus Obermayer, Gary G. Blasdel, and Klaus Schulten. Statistical-mechanical analysis of self-organization and pattern formation during the development of visual maps. *Phys. Rev. A*, 45:7568–7589, 1992.
- [168] Jörg A. Walter and Klaus Schulten. Implementation of self-organizing neural networks for visuo-motor control of an industrial robot. *IEEE Trans. Neur. Netw.*, 4:86–95, 1993.

- [169] Feng Zhou, Andreas Windemuth, and Klaus Schulten. Molecular dynamics study of the proton pump cycle of bacteriorhodopsin. *Biochemistry*, 32:2291–2306, 1993.
- [170] Klaus Obermayer, Klaus Schulten, and Gary G. Blasdel. A comparison between a neural network model for the formation of brain maps and experimental data. In D. S. Touretzky and R. Lippman, editors, *Advances in Neural Information Processing Systems 4*, pp. 83–90. Morgan Kaufmann Publishers, 1992.
- [171] Helmut Heller and Klaus Schulten. Parallel distributed computing for molecular dynamics: Simulation of large heterogeneous systems on a systolic ring of transputers. *Chem. Des. Autom. News*, 7:11–22, 1992.
- [172] Daniel Barsky, Benno Pütz, Klaus Schulten, J. Schoeniger, E. W. Hsu, and S. Blackband. Diffusional edge enhancement observed by NMR in thin glass capillaries. *Chem. Phys. Lett.*, 200:88–96, 1992.
- [173] John A. Board, Jr., J. W. Causey, James F. Leathrum, Jr., Andreas Windemuth, and Klaus Schulten. Accelerated molecular dynamics simulation with the parallel fast multipole algorithm. *Chem. Phys. Lett.*, 198:89–94, 1992.
- [174] Amitabh B. Sinha, Klaus Schulten, and Helmut Heller. Performance analysis of a parallel molecular dynamics program. *Comput. Phys. Commun.*, 78:265–278, 1994.
- [175] Ted Hesselroth, Kakali Sarkar, P. Patrick van der Smagt, and Klaus Schulten. Neural network control of a pneumatic robot arm. *IEEE Trans. Sys., Man, Cybern.*, 24:28–37, 1994.
- [176] Dong Xu and Klaus Schulten. Multi-mode coupling of protein motion to electron transfer in the photosynthetic reaction center: Spin-boson theory based on a classical molecular dynamics simulation. In J. Breton and A. Vermeglio, editors, *The Photosynthetic Bacterial Reaction Center: II. Structure, Spectroscopy and Dynamics*, NATO Sci. Ser. A, pp. 301–312. Plenum Press, New York, 1992.
- [177] Christian Kurrer and Klaus Schulten. Dependence of percolation thresholds on lattice connectivity. *Phys. Rev. E*, 48:614–617, 1993.
- [178] Thomas Martinetz and Klaus Schulten. Topology representing networks. *Neur. Netw.*, 7:507–522, 1994.
- [179] Helmut Heller, Michael Schaefer, and Klaus Schulten. Molecular dynamics simulation of a bilayer of 200 lipids in the gel and in the liquid crystal-phases. *J. Phys. Chem.*, 97:8343–8360, 1993.
- [180] Edgar Erwin, Klaus Obermayer, and Klaus Schulten. A comparison of models of visual cortical map formation. In Frank H. Eeckman and James M. Bower, editors, *Computation and Neural Systems*, chapter 60, pp. 395–402. Kluwer Academic Publishers, 1993.
- [181] Patrick van der Smagt and Klaus Schulten. Control of pneumatic robot arm dynamics by a neural network. In *Proceedings of the World Congress on Neural Networks, Portland, OR, July 11-15*, volume 3, pp. 180–183, 1993.
- [182] Thomas Martinetz and Klaus Schulten. A neural network with Hebbian-like adaptation rules learning visuomotor coordination of a PUMA robot. In *Proceedings of the IEEE International Conference on Neural Networks (ICNN-93), San Francisco*, pp. 820–825, 1993.
- [183] Kakali Sarkar and Klaus Schulten. Topology representing network in robotics. In J. Leo van Hemmen, Eytan Domany, and Klaus Schulten, editors, *Models of Neural Networks*, volume 3 of *Physics of Neural Networks*, pp. 281–302. Springer-Verlag, New York, 1996.
- [184] Benno Pütz, Daniel Barsky, and Klaus Schulten. Mechanisms of liposomal contrast agents in magnetic resonance imaging. *J. Liposome Res.*, 4:771–808, 1994.
- [185] William Humphrey, Ilya Logunov, Klaus Schulten, and Mordechai Sheves. Molecular dynamics study of bacteriorhodopsin and artificial pigments. *Biochemistry*, 33:3668–3678, 1994.

- [186] Thomas C. Bishop and Klaus Schulten. Molecular dynamics study of a sequence specific protein–DNA interaction. In G. Wipff, editor, *Computational Approaches in Supramolecular Chemistry*, pp. 419–439. Kluwer Academic Publishers, Boston, 1994.
- [187] Jeff M. Canfield, R. Linn Belford, Peter G. Debrunner, and Klaus Schulten. A perturbation theory treatment of oscillating magnetic fields in the radical pair mechanism. *Chem. Phys.*, 182:1–18, 1994.
- [188] Thomas C. Bishop, Helmut Heller, and Klaus Schulten. Molecular dynamics on parallel computers: Applications for theoretical biophysics. In Rajiv K. Kalia and Priya Vashishta, editors, *Toward Teraflop Computing and New Grand Challenge Applications*, pp. 129–138. Nova Science Publishers, Inc., New York, 1995.
- [189] Edgar Erwin, Klaus Obermayer, and Klaus Schulten. A critical comparison of models for orientation and ocular dominance columns in the striate cortex. In G. Tesauero, D. Touretzky, and T. Leen, editors, *Advances in Neural Information Processing Systems 7*, pp. 93–100. MIT Press, Cambridge, Mass and London, England, 1995.
- [190] Svilen Tzonev, Joseph Malpeli, and Klaus Schulten. Morphogenesis of the lateral geniculate nucleus: How singularities affect global structure. In G. Tesauero, D. Touretzky, and T. Leen, editors, *Advances in Neural Information Processing Systems 7*, pp. 133–140, Cambridge, Mass and London, England, 1995. MIT Press.
- [191] Edgar Erwin, Klaus Obermayer, and Klaus Schulten. Models of orientation and ocular dominance columns in the visual cortex: A critical comparison. *Neur. Comp.*, 7:425–468, 1995.
- [192] Ilya Logunov, William Humphrey, Klaus Schulten, and Mordechai Sheves. Molecular dynamics study of the 13-*cis* form (bR₅₄₈) of bacteriorhodopsin and its photocycle. *Biophys. J.*, 68:1270–1282, 1995.
- [193] Feng Zhou and Klaus Schulten. Molecular dynamics study of a membrane–water interface. *J. Phys. Chem.*, 99:2194–2208, 1995.
- [194] Christian Kurrer and Klaus Schulten. Noise-induced neuronal oscillations. *Phys. Rev. E*, 51:6213–6218, 1995.
- [195] Mark Nelson, William Humphrey, Attila Gursoy, Andrew Dalke, Laxmikant Kalé, Robert Skeel, Klaus Schulten, and Richard Kufin. MDScope – A visual computing environment for structural biology. *Comput. Phys. Commun.*, 91:111–134, 1995.
- [196] John A. Board, Jr., Laxmikant V. Kalé, Klaus Schulten, Robert D. Skeel, and Tamar Schlick. Modeling biomolecules: Larger scales, longer durations. *IEEE Comp. Sci. Eng.*, Winter:19–30, 1994.
- [197] James Phillips and Klaus Schulten. Modeling AFM tip dynamics through diffusion in time-periodic potentials. Beckman Institute Technical Report TB-95-03, University of Illinois, 1995.
- [198] Qing Sheng, Klaus Schulten, and Charles Pidgeon. A molecular dynamics simulation of immobilized artificial membranes. *J. Phys. Chem.*, 99:11018–11027, 1995.
- [199] Dong Xu, Klaus Schulten, Oren M. Becker, and Martin Karplus. Temperature quench echoes in proteins. *J. Chem. Phys.*, 103:3112–3123, 1995.
- [200] Dong Xu and Klaus Schulten. Velocity reassignment echoes in proteins. *J. Chem. Phys.*, 103:3124–3139, 1995.
- [201] Ioan Kosztin, Byron Faber, and Klaus Schulten. Introduction to the diffusion Monte Carlo method. *Am. J. Phys.*, 64:633–644, 1996.

- [202] Xiche Hu, Dong Xu, Kenneth Hamer, Klaus Schulten, Jürgen Koepke, and Hartmut Michel. Knowledge-based structure prediction of the light-harvesting complex II of *Rhodospirillum molischianum*. In P. M. Pardalos, D. Shalloway, and G. Xue, editors, *Global Minimization of Nonconvex Energy Functions: Molecular Conformation and Protein Folding*, pp. 97–122. American Mathematical Society, Providence, R.I., 1996.
- [203] Xiche Hu, Dong Xu, Kenneth Hamer, Klaus Schulten, Jürgen Koepke, and Hartmut Michel. Prediction of the structure of an integral membrane protein—the light-harvesting complex II of *Rhodospirillum molischianum*. In K.M. Merz and B. Roux, editors, *Biological Membranes: A Molecular Perspective from Computation and Experiment*, pp. 503–533. Birkhäuser, Cambridge, MA, 1996.
- [204] K.-R. Müller, M. Finke, N. Murata, K. Schulten, and S. Amari. Large scale simulations for learning curves. In Jong-Hoon Oh, Chulan Kwon, and Sungzoon Cho, editors, *Progress in neural Processing Vol. 1 / Neural Networks: The Statistical Mechanics Perspective*, pp. 73–84. World Scientific, Singapore, 1995.
- [205] Jeff M. Canfield, R. Linn Belford, Peter G. Debrunner, and Klaus Schulten. A perturbation theory treatment of oscillating magnetic fields in the radical pair mechanism - Erratum. *Chem. Phys.*, 191:347–347, 1995.
- [206] James Phillips and Klaus Schulten. Diffusive hysteresis at high and low driving frequencies. *Phys. Rev. E*, 52:2473–2477, 1995.
- [207] Mark Nelson, William Humphrey, Attila Gursoy, Andrew Dalke, Laxmikant Kalé, Robert Skeel, Klaus Schulten, and Richard Kufrin. MDSCOPE – A visual computing environment for structural biology. In S.N. Atluri, G. Yagawa, and T.A. Cruse, editors, *Computational Mechanics 95*, volume 1, pp. 476–481, 1995.
- [208] Xiche Hu, Dong Xu, Kenneth Hamer, Klaus Schulten, Jürgen Koepke, and Hartmut Michel. Predicting the structure of the light-harvesting complex II of *Rhodospirillum molischianum*. *Prot. Sci.*, 4:1670–1682, 1995.
- [209] Thomas C. Bishop and Klaus Schulten. Molecular dynamics study of glucocorticoid receptor–DNA binding. *Proteins: Struct., Func., Gen.*, 24:115–133, 1996.
- [210] Klaus Schulten, William Humphrey, Ilya Logunov, Mordechai Sheves, and Dong Xu. Molecular dynamics studies of bacteriorhodopsin’s photocycles. *Israel J. Chem.*, 35:447–464, 1995.
- [211] William Humphrey, Dong Xu, Mordechai Sheves, and Klaus Schulten. Molecular dynamics study of the early intermediates in the bacteriorhodopsin photocycle. *J. Phys. Chem.*, 99:14549–14560, 1995.
- [212] Michael Zeller, K. R. Wallace, and Klaus Schulten. Biological visuo-motor control of a pneumatic robot arm. In Dagli et al., editors, *Intelligent Engineering Systems Through Artificial Neural Networks*, volume 5, pp. 645–650, New York, 1995. American Society of Mechanical Engineers.
- [213] Ilya Logunov and Klaus Schulten. Quantum chemistry of *in situ* retinal: Study of the spectral properties and dark adaptation of bacteriorhodopsin. In D. Bicout and M. J. Field, editors, *Proceedings of the Ecole de Physique des Houches*, pp. 235–256, Paris, 1995. Les Editions de Physique, Springer.
- [214] Klaus Schulten. Curve crossing in a protein: Coupling of the elementary quantum process to motions of the protein. In D. Bicout and M. J. Field, editors, *Proceedings of the Ecole de Physique des Houches*, pp. 85–118, Paris, 1995. Les Editions de Physique, Springer.
- [215] J. M. Canfield, R. L. Belford, P. G. Debrunner, and K. Schulten. A perturbation treatment of oscillating magnetic fields in the radical pair mechanism using the Liouville equation. *Chem. Phys.*, 195:59–69, 1995.

- [216] Dong Xu, Mordechai Sheves, and Klaus Schulten. Molecular dynamics study of the M_{412} intermediate of bacteriorhodopsin. *Biophys. J.*, 69:2745–2760, 1995.
- [217] Klaus Schulten and Michael Zeller. Topology representing maps and brain function. In *Nova Acta Leopoldina NF*, volume 72, pp. 133–157. Jahresversammlungsband, 1996.
- [218] Dong Xu, Charles Martin, and Klaus Schulten. Molecular dynamics study of early picosecond events in the bacteriorhodopsin photocycle: Dielectric response, vibrational cooling and the J, K intermediates. *Biophys. J.*, 70:453–460, 1996.
- [219] K.-R. Müller, N. Murata, M. Finke, K. Schulten, and S. Amari. A numerical study of learning curves in stochastic multi-layer feed-forward networks. *Neur. Comp.*, 8:1085–1106, 1995.
- [220] Manel A. Balsera, Willy Wriggers, Yoshitsugu Oono, and Klaus Schulten. Principal component analysis and long time protein dynamics. *J. Phys. Chem.*, 100:2567–2572, 1996.
- [221] Klaus Schulten, Hui Lu, and Linsen Bai. Probing protein motion through temperature echoes. In Henrik Flyvbjerg, John Hertz, Mogens H. Jensen, Ole G. Mouritsen, and Kim Sneppen, editors, *Physics of Biological Systems: From Molecules to Species*, Lecture Notes in Physics, pp. 117–152. Springer, 1997.
- [222] William Humphrey, Andrew Dalke, and Klaus Schulten. VMD – Visual Molecular Dynamics. *J. Mol. Graphics*, 14:33–38, 1996.
- [223] Feng Zhou and Klaus Schulten. Molecular dynamics study of the activation of phospholipase A_2 on a membrane surface. *Proteins: Struct., Func., Gen.*, 25:12–27, 1996.
- [224] Dong Xu, James Christopher Phillips, and Klaus Schulten. Protein response to external electric fields: Relaxation, hysteresis, and echo. *J. Phys. Chem.*, 100:12108–12121, 1996.
- [225] Juergen Koepke, Xiche Hu, Cornelia Muenke, Klaus Schulten, and Hartmut Michel. The crystal structure of the light harvesting complex II (B800-850) from *Rhodospirillum rubrum*. *Structure*, 4:581–597, 1996.
- [226] Mark Nelson, William Humphrey, Attila Gursoy, Andrew Dalke, Laxmikant Kalé, Robert D. Skeel, and Klaus Schulten. NAMD – A parallel, object-oriented molecular dynamics program. *Int. J. Supercomp. Appl. High Perform. Comp.*, 10:251–268, 1996.
- [227] R. Sharma, T. S. Huang, V. I. Pavlovic, K. Schulten, A. Dalke, J. Phillips, M. Zeller, W. Humphrey, Y. Zhao, Z. Lo, and S. Chu. Speech/gesture interface to a visual computing environment for molecular biologists. In *Proceedings of 13th ICPR 96*, volume 3, pp. 964–968, 1996.
- [228] Ilya Logunov and Klaus Schulten. Quantum chemistry – molecular dynamics study of the dark adaptation process in bacteriorhodopsin. *J. Am. Chem. Soc.*, 118:9727–9735, 1996.
- [229] Michael Zeller, Rajeev Sharma, and Klaus Schulten. Topology representing network for sensor-based robot motion planning. In *Proceedings of the 1996 World Congress on Neural Networks*, pp. 100–103. INNS Press, 1996.
- [230] Michael Zeller, Rajeev Sharma, and Klaus Schulten. Vision-based motion planning of a pneumatic robot using a topology representing neural network. In *Proceedings of 1996 IEEE Int. Symposium on Intelligent Control*, pp. 7–12, 1996.
- [231] P. van der Smagt, F. Grön, and K. Schulten. Analysis and control of a rubber-tuator arm. *Biol. Cyber.*, 75:433–440, 1996.
- [232] Andrew Dalke and Klaus Schulten. Using TCL for molecular visualization and analysis. In *Proceedings of the Pacific Symposium on Biocomputing '97*, volume 2, pp. 85–96, 1997.

- [233] Daniel Barsky, Benno Pütz, and Klaus Schulten. Theory of heterogeneous relaxation in compartmentalized tissues. *Magn. Res. Med.*, 37:666–675, 1997.
- [234] William Humphrey, Ernst Bamberg, and Klaus Schulten. Photoproducts of bacteriorhodopsin mutants: A molecular dynamics study. *Biophys. J.*, 72:1347–1356, 1997.
- [235] Michael Zeller, Rajeev Sharma, and Klaus Schulten. Motion planning of a pneumatic robot using a neural network. *IEEE Control Systems Magazine*, 17:89–98, 1997.
- [236] Sergei Izrailev, Sergey Stepaniants, Manel Balsera, Yoshi Oono, and Klaus Schulten. Molecular dynamics study of unbinding of the avidin-biotin complex. *Biophys. J.*, 72:1568–1581, 1997.
- [237] Tom Connor Bishop, Dorina Kosztin, and Klaus Schulten. How hormone receptor–DNA binding affects nucleosomal DNA: The role of symmetry. *Biophys. J.*, 72:2056–2067, 1997.
- [238] Michael Zeller, Rajeev Sharma, and Klaus Schulten. Vision-based robot motion planning using a topology representing neural network. In Jens Kalkkuhl, Ken Hunt, Rafal Zbikowski, and Andrzej Dzielinski, editors, *Applications of Neural Adaptive Control Technology*, volume 17 of *World Scientific Series in Robotics and Intelligent Systems*, pp. 181–204. World Scientific Publishing, 1997.
- [239] Ioan Kosztin and Klaus Schulten. Boundary integral method for stationary states of two-dimensional quantum systems. *Int. J. of Modern Phys. C*, 8:293–325, 1997.
- [240] Xiche Hu, Thorsten Ritz, Ana Damjanović, and Klaus Schulten. Pigment organization and transfer of electronic excitation in the purple bacteria. *J. Phys. Chem. B*, 101:3854–3871, 1997.
- [241] Willy Wriggers and Klaus Schulten. Protein domain movements: Detection of rigid domains and visualization of hinges in comparisons of atomic coordinates. *Proteins: Struct., Func., Gen.*, 29:1–14, 1997.
- [242] Thomas C. Bishop, Robert D. Skeel, and Klaus Schulten. Difficulties with multiple time stepping and the fast multipole algorithm in molecular dynamics. *J. Comp. Chem.*, 18:1785–1791, 1997.
- [243] Dorina Kosztin, Thomas C. Bishop, and Klaus Schulten. Binding of the estrogen receptor to DNA: The role of waters. *Biophys. J.*, 73:557–570, 1997.
- [244] Manel Balsera, Sergey Stepaniants, Sergei Izrailev, Yoshitsugu Oono, and Klaus Schulten. Reconstructing potential energy functions from simulated force-induced unbinding processes. *Biophys. J.*, 73:1281–1287, 1997.
- [245] Willy Wriggers and Klaus Schulten. Stability and dynamics of G-actin: Back door water diffusion and behavior of a subdomain 3/4 loop. *Biophys. J.*, 73:624–639, 1997.
- [246] Michael Zeller, Rajeev Sharma, and Klaus Schulten. Learning the perceptual control manifold for sensor-based robot path planning. In *Proceedings of the 1997 IEEE International Symposium on Computational Intelligence in Robotics and Automation (CIRA '97)*, pp. 48–53. IEEE Computer Society Press, 1997.
- [247] Michael Zeller, James C. Phillips, Andrew Dalke, William Humphrey, Klaus Schulten, Rajeev Sharma, T. S. Huang, V. I. Pavlovic, Y. Zhao, Z. Lo, and S. Chu. A visual computing environment for very large scale biomolecular modeling. In *Proceedings of the 1997 IEEE International Conference on Application-specific Systems, Architectures and Processors (ASAP)*, pp. 3–12. IEEE Computer Society Press, 1997.
- [248] Xiche Hu and Klaus Schulten. How nature harvests sunlight. *Physics Today*, 50:28–34, 1997.
- [249] James C. Phillips, Willy Wriggers, Zhigang Li, Ana Jonas, and Klaus Schulten. Predicting the structure of apolipoprotein A-I in reconstituted high density lipoprotein disks. *Biophys. J.*, 73:2337–2346, 1997.

- [250] Barry Isralewitz, Sergei Izrailev, and Klaus Schulten. Binding pathway of retinal to bacterio-opsin: A prediction by molecular dynamics simulations. *Biophys. J.*, 73:2972–2979, 1997.
- [251] Sergey Stepaniants, Sergei Izrailev, and Klaus Schulten. Extraction of lipids from phospholipid membranes by steered molecular dynamics. *J. Mol. Mod.*, 3:473–475, 1997.
- [252] Ivo Hofacker and Klaus Schulten. Oxygen and proton pathways in cytochrome *c* oxidase. *Proteins: Struct., Func., Gen.*, 30:100–107, 1998.
- [253] Alexander Balaeff, Mair E. A. Churchill, and Klaus Schulten. Structure prediction of a complex between the chromosomal protein HMG-D and DNA. *Proteins: Struct., Func., Gen.*, 30:113–135, 1998.
- [254] Thorsten Ritz, Xiche Hu, Ana Damjanović, and Klaus Schulten. Excitons and excitation transfer in the photosynthetic unit of purple bacteria. *J. Luminesc.*, 76-77:310–321, 1998.
- [255] Sergei Izrailev, Sergey Stepaniants, Barry Isralewitz, Dorina Kosztin, Hui Lu, Ferenc Molnar, Willy Wriggers, and Klaus Schulten. Steered molecular dynamics. In P. Deuffhard, J. Hermans, B. Leimkuhler, A. E. Mark, S. Reich, and R. D. Skeel, editors, *Computational Molecular Dynamics: Challenges, Methods, Ideas*, volume 4 of *Lecture Notes in Computational Science and Engineering*, pp. 39–65. Springer-Verlag, Berlin, 1998.
- [256] James C. Phillips, Robert Brunner, Aritomo Shinozaki, Milind Bhandarkar, Neal Krawetz, Laxmikant Kalé, Robert D. Skeel, and Klaus Schulten. Avoiding algorithmic obfuscation in a message-driven parallel MD code. In P. Deuffhard, J. Hermans, B. Leimkuhler, A. Mark, S. Reich, and R. D. Skeel, editors, *Computational Molecular Dynamics: Challenges, Methods, Ideas*, volume 4 of *Lecture Notes in Computational Science and Engineering*, pp. 472–482. Springer-Verlag, 1998.
- [257] Svilen Tzonev, Joseph Malpeli, and Klaus Schulten. A three-dimensional model of the morphogenesis of the rhesus lateral geniculate nucleus. Beckman Institute Technical Report, University of Illinois, 1998.
- [258] Willy Wriggers and Klaus Schulten. Nucleotide-dependent movements of the kinesin motor domain predicted by simulated annealing. *Biophys. J.*, 75:646–661, 1998.
- [259] Xiche Hu, Ana Damjanović, Thorsten Ritz, and Klaus Schulten. Architecture and function of the light harvesting apparatus of purple bacteria. *Proc. Natl. Acad. Sci. USA*, 95:5935–5941, 1998.
- [260] Michael Bailey, Klaus Schulten, and John E. Johnson. The use of solid physical models for the study of macromolecular assembly. *Curr. Opin. Struct. Biol.*, 8:202–208, 1998.
- [261] Willy Wriggers, Ernest Mehler, Felicia Pitici, Harel Weinstein, and Klaus Schulten. Structure and dynamics of calmodulin in solution. *Biophys. J.*, 74:1622–1639, 1998.
- [262] Michal Ben-Nun, Ferenc Molnar, Hui Lu, James C. Phillips, Todd J. Martínez, and Klaus Schulten. Quantum dynamics of retinal’s femtosecond photoisomerization in bacteriorhodopsin. In *Faraday Discussions*, No. 110, pp. 447–462. Faraday Publications, 1998.
- [263] Xiche Hu and Klaus Schulten. A model for the light-harvesting complex I (B875) of *Rhodobacter sphaeroides*. *Biophys. J.*, 75:683–694, 1998.
- [264] Ana Damjanović, Thorsten Ritz, and Klaus Schulten. Energy transfer between carotenoids and bacteriochlorophylls in a light harvesting protein. *Phys. Rev. E*, 59:3293–3311, 1999.
- [265] Hui Lu, Barry Isralewitz, André Krammer, Viola Vogel, and Klaus Schulten. Unfolding of titin immunoglobulin domains by steered molecular dynamics simulation. *Biophys. J.*, 75:662–671, 1998.
- [266] W. Humphrey, H. Lu, I. Logunov, H. J. Werner, and K. Schulten. Three electronic state model of the primary phototransformation of bacteriorhodopsin. *Biophys. J.*, 75:1689–1699, 1998.

- [267] David Kaufman, Ioan Kosztin, and Klaus Schulten. Expansion method for stationary states of quantum billiards. *Am. J. Phys.*, 67:133–141, 1999.
- [268] Klaus Schulten. From simplicity to complexity and back: Function, architecture and mechanism of light harvesting systems in photosynthetic bacteria. In H. Frauenfelder, J. Deisenhofer, and P. G. Wolynes, editors, *Simplicity and Complexity in Proteins and Nucleic Acids*, pp. 227–253, Berlin, 1999. Dahlem University Press. (pdf available from author upon request).
- [269] Marshall G. Cory, Michael C. Zerner, Xiche Hu, and Klaus Schulten. Electronic excitations in aggregates of bacteriochlorophylls. *J. Phys. Chem. B*, 102:7640–7650, 1998.
- [270] Dorina Kosztin, Sergei Izrailev, and Klaus Schulten. Unbinding of retinoic acid from its receptor studied by steered molecular dynamics. *Biophys. J.*, 76:188–197, 1999.
- [271] Thorsten Ritz, Ana Damjanović, and Klaus Schulten. Light-harvesting and photoprotection by carotenoids: Structure-based calculations for photosynthetic antenna systems. In G. Garab, editor, *Photosynthesis: Mechanisms and Effects (Proceedings of the XIth International Congress on Photosynthesis)*, volume 1, pp. 487–490, Dordrecht, 1998. Kluwer Academic Publications.
- [272] Milind Bhandarkar, Gila Budescu, William Humphrey, Jesus A. Izaguirre, Sergei Izrailev, Laxmikant V. Kalé, Dorina Kosztin, Ferenc Molnar, James C. Phillips, and Klaus Schulten. BioCoRE: A laboratory for structural biology. In Agostino G. Bruzzone, Adelinde Uchrmacher, and Ernest H. Page, editors, *Proceedings of the SCS International Conference on Web-Based Modeling and Simulation*, pp. 242–251, San Francisco, California, 1999.
- [273] Willy Wriggers, Ronald A. Milligan, Klaus Schulten, and J. Andrew McCammon. Self-organizing neural networks bridge the biomolecular resolution gap. *J. Mol. Biol.*, 284:1247–1254, 1998.
- [274] Willy Wriggers and Klaus Schulten. Investigating a back door mechanism of actin phosphate release by steered molecular dynamics. *Proteins: Struct., Func., Gen.*, 35:262–273, 1999.
- [275] Justin Gullingsrud, Rosemary Braun, and Klaus Schulten. Reconstructing potentials of mean force through time series analysis of steered molecular dynamics simulations. *J. Comp. Phys.*, 151:190–211, 1999.
- [276] Laxmikant Kalé, Robert Skeel, Milind Bhandarkar, Robert Brunner, Attila Gursoy, Neal Krawetz, James Phillips, Aritomo Shinozaki, Krishnan Varadarajan, and Klaus Schulten. NAMD2: Greater scalability for parallel molecular dynamics. *J. Comp. Phys.*, 151:283–312, 1999.
- [277] André Krammer, Hui Lu, Barry Isralewitz, Klaus Schulten, and Viola Vogel. Forced unfolding of the fibronectin type III module reveals a tensile molecular recognition switch. *Proc. Natl. Acad. Sci. USA*, 96:1351–1356, 1999.
- [278] Tamar Schlick, Robert Skeel, Axel Brünger, Laxmikant Kalé, John A. Board Jr., Jan Hermans, and Klaus Schulten. Algorithmic challenges in computational molecular biophysics. *J. Comp. Phys.*, 151:9–48, 1999.
- [279] Hui Lu and Klaus Schulten. Steered molecular dynamics simulations of force-induced protein domain unfolding. *Proteins: Struct., Func., Gen.*, 35:453–463, 1999.
- [280] Christian V. Forst and Klaus Schulten. Evolution of metabolisms: A new method for the comparison of metabolic pathways. In Sorin Istrail, Pavel Pevzner, and Michael Waterman, editors, *Proceedings of the Third Annual International Conference on Computational Molecular Biology*, pp. 174–180, Lyon, France, 1999. ACM Press, New York.
- [281] Hui Lu and Klaus Schulten. Steered molecular dynamics simulation of conformational changes of immunoglobulin domain I27 interpret atomic force microscopy observations. *Chem. Phys.*, 247:141–153, 1999.

- [282] Dorina Kosztin, Richard Gumport, and Klaus Schulten. Probing the role of structural water in a duplex oligodeoxyribonucleotide containing a water-mimicking base analogue. *Nucleic Acids Res.*, 27:3550–3556, 1999.
- [283] Sergei Izrailev, Antony R. Crofts, Edward A. Berry, and Klaus Schulten. Steered molecular dynamics simulation of the Rieske subunit motion in the cytochrome bc_1 complex. *Biophys. J.*, 77:1753–1768, 1999.
- [284] Hui Lu, André Krammer, Barry Isralewitz, Viola Vogel, and Klaus Schulten. Computer modeling of force-induced titin domain unfolding. In Jerry Pollack and Henk Granzier, editors, *Elastic Filaments of the Cell*, chapter 1, pp. 143–162. Kluwer Academic/Plenum Publishers, New York, NY, 2000.
- [285] Emad Tajkhorshid, Jerome Baudry, Klaus Schulten, and Sandor Suhai. Molecular dynamics study of the nature and origin of retinal’s twisted structure in bacteriorhodopsin. *Biophys. J.*, 78:683–693, 2000.
- [286] Piotr E. Marszalek, Hui Lu, Hongbin Li, Mariano Carrion-Vazquez, Andres F. Oberhauser, Klaus Schulten, and Julio M. Fernandez. Mechanical unfolding intermediates in titin modules. *Nature*, 402:100–103, 1999.
- [287] Thorsten Ritz, Salih Adem, and Klaus Schulten. A model for photoreceptor-based magnetoreception in birds. *Biophys. J.*, 78:707–718, 2000.
- [288] Ana Damjanović, Thorsten Ritz, and Klaus Schulten. Excitation energy trapping by the reaction center of *Rhodobacter sphaeroides*. *Int. J. Quantum Chem.*, 77:139–151, 2000.
- [289] Christian Forst and Klaus Schulten. Evolution of metabolisms: A new method for the comparison of metabolic pathways using genomics information. *Journal of Computational Biology*, 6:343–360, 1999.
- [290] Alexander Balaeff, L. Mahadevan, and Klaus Schulten. Elastic rod model of a DNA loop in the *lac* operon. *Phys. Rev. Lett.*, 83:4900–4903, 1999.
- [291] K. Moffat, J.-P. Changeux, D. M. Crothers, H. Grubmueller, G. U. Nienhaus, M. U. Palma, F. G. Parak, K. Schulten, and A. Warshel. Group report: How does complexity lead to an apparently simple function? In H. Frauenfelder, J. Deisenhofer, and P. G. Wolynes, editors, *Simplicity and Complexity in Proteins and Nucleic Acids*, pp. 255–280, Berlin, 1999. Dahlem University Press.
- [292] John Board and Klaus Schulten. The fast multipole algorithm. *IEEE Comp. Sci. Eng.*, 2:56–59, 2000.
- [293] Ferenc Molnar, Michal Ben-Nun, Todd J. Martínez, and Klaus Schulten. Characterization of a conical intersection between the ground and first excited state for a retinal analog. *J. Mol. Struct. (THEOCHEM)*, WATOC special issue, 506:169–178, 2000.
- [294] Rajeev Sharma, Michael Zeller, Vladimir I. Pavlovic, Thomas S. Huang, Zion Lo, Stephen Chu, Yunxin Zhao, James C. Phillips, and Klaus Schulten. Speech/gesture interface to a visual-computing environment. *IEEE Comp. Graph. App.*, 20:29–37, 2000.
- [295] Ferenc Molnar, Lawrence S. Norris, and Klaus Schulten. Simulated unbinding and binding of fatty acid substrates in the cyclooxygenase site of prostaglandin H_2 synthase-1. *Progr. React. Kin. Mech.*, 25:263–298, 2000.
- [296] Ana Damjanović, Thorsten Ritz, and Klaus Schulten. Excitation transfer in the peridinin-chlorophyll-protein of *Amphidinium carterae*. *Biophys. J.*, 79:1695–1705, 2000.
- [297] Klaus Schulten. Electron transfer: Exploiting thermal motion. *Science*, 290:61–62, 2000.
- [298] Amit Kessel, Klaus Schulten, and Nir Ben-Tal. Calculations suggest a pathway for the transverse diffusion of a hydrophobic peptide across a lipid bilayer. *Biophys. J.*, 79:2322–2330, 2000.

- [299] Klaus Schulten. To students contemplating research in biomolecular modelling. *Journal of Molecular Graphics and Modeling*, 18:218–220, 2000.
- [300] Hui Lu and Klaus Schulten. The key event in force-induced unfolding of titin’s immunoglobulin domains. *Biophys. J.*, 79:51–65, 2000.
- [301] Thorsten Ritz, Ana Damjanović, Klaus Schulten, Jian-Ping Zhang, and Yasushi Koyama. Efficient light harvesting through carotenoids. *Photosyn. Res.*, 66:125–144, 2000.
- [302] Jerome Baudry, Emad Tajkhorshid, Ferenc Molnar, James Phillips, and Klaus Schulten. Molecular dynamics study of bacteriorhodopsin and the purple membrane. *J. Phys. Chem. B*, 105:905–918, 2001.
- [303] Barry Isralewitz, Jerome Baudry, Justin Gullingsrud, Dorina Kosztin, and Klaus Schulten. Steered molecular dynamics investigations of protein function. *Journal of Molecular Graphics and Modeling*, 19:13–25, 2001. Also in *Protein Flexibility and Folding*, L. A. Kuhn and M. F. Thorpe, editors, *Biological Modeling Series* (Elsevier).
- [304] John E. Stone, Justin Gullingsrud, Paul Grayson, and Klaus Schulten. A system for interactive molecular dynamics simulation. In John F. Hughes and Carlo H. Séquin, editors, *2001 ACM Symposium on Interactive 3D Graphics*, pp. 191–194, New York, 2001. ACM SIGGRAPH.
- [305] Christian Forst and Klaus Schulten. Phylogenetic analysis of metabolic pathways. *Journal of Molecular Evolution*, 52:471–489, 2001.
- [306] Thorsten Ritz and Klaus Schulten. Physik der Photosynthese. *Physikalische Blätter*, 57:49–53, 2001.
- [307] Barry Isralewitz, Mu Gao, and Klaus Schulten. Steered molecular dynamics and mechanical functions of proteins. *Curr. Opin. Struct. Biol.*, 11:224–230, 2001.
- [308] Justin Gullingsrud, Dorina Kosztin, and Klaus Schulten. Structural determinants of MscL gating studied by molecular dynamics simulations. *Biophys. J.*, 80:2074–2081, 2001.
- [309] David Craig, André Krammer, Klaus Schulten, and Viola Vogel. Comparison of the early stages of forced unfolding of fibronectin type III modules. *Proc. Natl. Acad. Sci. USA*, 98:5590–5595, 2001.
- [310] Mu Gao, Hui Lu, and Klaus Schulten. Simulated refolding of stretched titin immunoglobulin domains. *Biophys. J.*, 81:2268–2277, 2001.
- [311] Thorsten Ritz, Sanghyun Park, and Klaus Schulten. Kinetics of excitation migration and trapping in the photosynthetic unit of purple bacteria. *J. Phys. Chem. B*, 105:8259–8267, 2001.
- [312] Shigehiko Hayashi, Emad Tajkhorshid, Eva Pebay-Peyroula, Antoine Royant, Ehud M. Landau, Javier Navarro, and Klaus Schulten. Structural determinants of spectral tuning in retinal proteins – bacteriorhodopsin vs sensory rhodopsin II. *J. Phys. Chem. B*, 105:10124–10131, 2001.
- [313] Fangqiang Zhu, Emad Tajkhorshid, and Klaus Schulten. Molecular dynamics study of aquaporin-1 water channel in a lipid bilayer. *FEBS Lett.*, 504:212–218, 2001.
- [314] Thomas W. Lynch, Dorina Kosztin, Mark A. McLean, Klaus Schulten, and Stephen G. Sligar. Dissecting the molecular origins of protein-nucleic acid recognition: Hydrostatic pressure and molecular dynamics. *Biophys. J.*, 82:93–98, 2002.
- [315] Melih Şener and Klaus Schulten. A general random matrix approach to account for the effect of static disorder on the spectral properties of light harvesting systems. *Phys. Rev. E*, 65:031916, 2002. (12 pages).
- [316] Thorsten Ritz, Ana Damjanović, and Klaus Schulten. The quantum physics of photosynthesis. *ChemPhysChem*, 3:243–248, 2002.

- [317] Xiche Hu, Thorsten Ritz, Ana Damjanović, Felix Autenrieth, and Klaus Schulten. Photosynthetic apparatus of purple bacteria. *Quart. Rev. Biophys.*, 35:1–62, 2002.
- [318] Morten Ø. Jensen, Emad Tajkhorshid, and Klaus Schulten. The mechanism of glycerol conduction in aquaglyceroporins. *Structure*, 9:1083–1093, 2001.
- [319] André Krammer, David Craig, Wendy E. Thomas, Klaus Schulten, and Viola Vogel. A structural model for force regulated integrin binding to fibronectin’s RGD-synergy site. *Matrix Biology*, 21:139–147, 2002.
- [320] Ana Damjanović, Ioan Kosztin, Ulrich Kleinekathoefer, and Klaus Schulten. Excitons in a photosynthetic light-harvesting system: A combined molecular dynamics, quantum chemistry and polaron model study. *Phys. Rev. E*, 65:031919, 2002. (24 pages).
- [321] Michal Ben-Nun, Ferenc Molnar, Klaus Schulten, and Todd J. Martinez. The role of intersection topography in bond selectivity of *cis-trans* photoisomerization. *Proc. Natl. Acad. Sci. USA*, 99:1769–1773, 2002.
- [322] Rob Phillips, Markus Dittrich, and Klaus Schulten. Quasicontinuum representations of atomic-scale mechanics: From proteins to dislocations. *Annu. Rev. Mater. Res.*, 32:219–233, 2002.
- [323] Ioan Kosztin, Robijn Bruinsma, Paul O’Lague, and Klaus Schulten. Mechanical force generation by G-proteins. *Proc. Natl. Acad. Sci. USA*, 99:3575–3580, 2002.
- [324] Thomas W. Lynch, Mark A. McLean, Dorina Kosztin, Klaus Schulten, and Stephen G. Sligar. High pressure gel mobility shift analysis and molecular dynamics: Investigating specific protein-nucleic acid recognition. In R. Hayashi, editor, *Trends in High Pressure Bioscience and Biotechnology*, pp. 87–94. Elsevier, 2002.
- [325] Shigehiko Hayashi, Emad Tajkhorshid, and Klaus Schulten. Structural changes during the formation of early intermediates in the bacteriorhodopsin photocycle. *Biophys. J.*, 83:1281–1297, 2002.
- [326] John Ervin, Edgar Larios, Szabolcs Osvath, Klaus Schulten, and Martin Gruebele. What causes hyperfluorescence: folding intermediates or conformationally flexible native states? *Biophys. J.*, 83:473–483, 2002.
- [327] Fangqiang Zhu, Emad Tajkhorshid, and Klaus Schulten. Pressure-induced water transport in membrane channels studied by molecular dynamics. *Biophys. J.*, 83:154–160, 2002.
- [328] Morten O. Jensen, Sanghyun Park, Emad Tajkhorshid, and Klaus Schulten. Energetics of glycerol conduction through aquaglyceroporin GlpF. *Proc. Natl. Acad. Sci. USA*, 99:6731–6736, 2002.
- [329] Emad Tajkhorshid, Peter Nollert, Morten O. Jensen, Larry J. W. Miercke, Joseph O’Connell, Robert M. Stroud, and Klaus Schulten. Control of the selectivity of the aquaporin water channel family by global orientational tuning. *Science*, 296:525–530, 2002.
- [330] Rosemary Braun, Mehmet Sarikaya, and Klaus Schulten. Genetically engineered gold-binding polypeptides: Structure prediction and molecular dynamics. *J. Biomat. Sci.*, 13:747–758, 2002.
- [331] Melih K. Şener, Deyu Lu, Thorsten Ritz, Sanghyun Park, Petra Fromme, and Klaus Schulten. Robustness and optimality of light harvesting in cyanobacterial photosystem I. *J. Phys. Chem. B*, 106:7948–7960, 2002.
- [332] Mu Gao, Matthias Wilmanns, and Klaus Schulten. Steered molecular dynamics studies of titin II domain unfolding. *Biophys. J.*, 83:3435–3445, 2002.
- [333] Jan Saam, Emad Tajkhorshid, Shigehiko Hayashi, and Klaus Schulten. Molecular dynamics investigation of primary photoinduced events in the activation of rhodopsin. *Biophys. J.*, 83:3097–3112, 2002.

- [334] Mu Gao, Hui Lu, and Klaus Schulten. Unfolding of titin domains studied by molecular dynamics simulations. *J. Muscle Res. Cell Mot.*, 23:513–521, 2002.
- [335] Mu Gao, David Craig, Viola Vogel, and Klaus Schulten. Identifying unfolding intermediates of FN-III₁₀ by steered molecular dynamics. *J. Mol. Biol.*, 323:939–950, 2002.
- [336] M. V. Bayas, Klaus Schulten, and D. Leckband. Forced detachment of the CD2-CD58 complex. *Biophys. J.*, 84:2223–2233, 2003.
- [337] Paul Grayson, Emad Tajkhorshid, and Klaus Schulten. Mechanisms of selectivity in channels and enzymes studied with interactive molecular dynamics. *Biophys. J.*, 85:36–48, 2003.
- [338] Fangqiang Zhu and Klaus Schulten. Water and proton conduction through carbon nanotubes as models for biological channels. *Biophys. J.*, 85:236–244, 2003.
- [339] Sanghyun Park, Melih K. Şener, Deyu Lu, and Klaus Schulten. Reaction paths based on mean first-passage times. *J. Chem. Phys.*, 119:1313–1319, 2003.
- [340] Emad Tajkhorshid, Aleksij Aksimentiev, Ilya Balabin, Mu Gao, Barry Isralewitz, James C. Phillips, Fangqiang Zhu, and Klaus Schulten. Large scale simulation of protein mechanics and function. In Frederic M. Richards, David S. Eisenberg, and John Kuriyan, editors, *Advances in Protein Chemistry*, volume 66, pp. 195–247. Elsevier Academic Press, New York, 2003.
- [341] Shigehiko Hayashi, Emad Tajkhorshid, and Klaus Schulten. Molecular dynamics simulation of bacteriorhodopsin’s photoisomerization using *ab initio* forces for the excited chromophore. *Biophys. J.*, 85:1440–1449, 2003.
- [342] Sanghyun Park, Fatemeh Khalili-Araghi, Emad Tajkhorshid, and Klaus Schulten. Free energy calculation from steered molecular dynamics simulations using Jarzynski’s equality. *J. Chem. Phys.*, 119:3559–3566, 2003.
- [343] Justin Gullingsrud and Klaus Schulten. Gating of MscL studied by steered molecular dynamics. *Biophys. J.*, 85:2087–2099, 2003.
- [344] Morten Ø. Jensen, Emad Tajkhorshid, and Klaus Schulten. Electrostatic tuning of permeation and selectivity in aquaporin water channels. *Biophys. J.*, 85:2884–2899, 2003.
- [345] Deyu Lu, Paul Grayson, and Klaus Schulten. Glycerol conductance and physical asymmetry of the *Escherichia coli* glycerol facilitator GlpF. *Biophys. J.*, 85:2977–2987, 2003.
- [346] Markus Dittrich, Shigehiko Hayashi, and Klaus Schulten. On the mechanism of ATP hydrolysis in F₁-ATPase. *Biophys. J.*, 85:2253–2266, 2003.
- [347] Mu Gao, David Craig, Olivier Lequin, Iain D. Campbell, Viola Vogel, and Klaus Schulten. Structure and functional significance of mechanically unfolded fibronectin type III₁ intermediates. *Proc. Natl. Acad. Sci. USA*, 100:14784–14789, 2003.
- [348] Mehmet Sarikaya, Candan Tamerler, Alex K. -Y. Jen, Klaus Schulten, and François Baneyx. Molecular biomimetics: nanotechnology through biology. *Nature Materials*, 2:577–585, 2003.
- [349] Alexander Balaeff, L. Mahadevan, and Klaus Schulten. Structural basis for cooperative DNA binding by CAP and *Lac* repressor. *Structure*, 12:123–132, 2004.
- [350] Fangqiang Zhu, Emad Tajkhorshid, and Klaus Schulten. Theory and simulation of water permeation in aquaporin-1. *Biophys. J.*, 86:50–57, 2004.
- [351] David Craig, Mu Gao, Klaus Schulten, and Viola Vogel. Tuning the mechanical stability of fibronectin type III modules through sequence variation. *Structure*, 12:21–30, 2004.

- [352] Aleksij Aksimentiev, Ilya A. Balabin, Robert H. Fillingame, and Klaus Schulten. Insights into the molecular mechanism of rotation in the Fo sector of ATP synthase. *Biophys. J.*, 86:1332–1344, 2004.
- [353] Alexander Balaeff, Christophe R. Koudella, L. Mahadevan, and Klaus Schulten. Modeling DNA loops using continuum and statistical mechanics. *Phil. Trans. R. Soc. Lond. A*, 362:1355–1371, 2004.
- [354] Jordi Cohen and Klaus Schulten. Mechanism of anionic conduction across CLC. *Biophys. J.*, 86:836–845, 2004.
- [355] Boaz Ilan, Emad Tajkhorshid, Klaus Schulten, and Gregory A. Voth. The mechanism of proton exclusion in aquaporin channels. *Proteins: Struct., Func., Bioinf.*, 55:223–228, 2004.
- [356] Sanghyun Park and Klaus Schulten. Calculating potentials of mean force from steered molecular dynamics simulations. *J. Chem. Phys.*, 120:5946–5961, 2004.
- [357] Justin Gullingsrud and Klaus Schulten. Lipid bilayer pressure profiles and mechanosensitive channel gating. *Biophys. J.*, 86:3496–3509, 2004.
- [358] Aleksij Aksimentiev and Klaus Schulten. Extending the molecular modeling methodology to study insertion of membrane nanopores. *Proc. Natl. Acad. Sci. USA*, 101:4337–4338, 2004.
- [359] Melih K. Şener, Sanghyun Park, Deyu Lu, Ana Damjanović, Thorsten Ritz, Petra Fromme, and Klaus Schulten. Excitation migration in trimeric cyanobacterial photosystem I. *J. Chem. Phys.*, 120:11183–11195, 2004.
- [360] E. Larios, J. S. Li, K. Schulten, H. Kihara, and M. Gruebele. Multiple probes reveal a native-like intermediate during the low-temperature refolding of ubiquitin. *J. Mol. Biol.*, 340:115–125, 2004.
- [361] Rosemary Braun, Donald M. Engelman, and Klaus Schulten. Molecular dynamics simulations of micelle formation around dimeric glycophorin A transmembrane helices. *Biophys. J.*, 87:754–763, 2004.
- [362] Elizabeth Villa, Alexander Balaeff, L. Mahadevan, and Klaus Schulten. Multi-scale method for simulating protein-DNA complexes. *Multiscale Model. Simul.*, 2:527–553, 2004.
- [363] Mu Gao and Klaus Schulten. Integrin activation in vivo and in silico. *Structure*, 12:2096–2098, 2004.
- [364] M. V. Bayas, K. Schulten, and D. Leckband. Forced dissociation of the strand dimer interface between C-cadherin ectodomains. *Mechanics and Chemistry of Biosystems*, 1:101–111, 2004.
- [365] Jerome Baudry, Emad Tajkhorshid, and Klaus Schulten. Complementarities and convergence of results in bacteriorhodopsin trimer simulations. *Biophys. J.*, 87:1394–1395, 2004.
- [366] Yan Li, Deyu Lu, Slava V. Rotkin, Klaus Schulten, and Umberto Ravaioli. Electronic structure and dielectric behavior of finite-length single-walled carbon nanotubes. In *Proceedings of the Fourth IEEE Conference on Nanotechnology*, pp. 273–275, Munich, Germany, 2004.
- [367] Edgar Larios, Wei Y. Yang, Klaus Schulten, and Martin Gruebele. A similarity measure for partially folded proteins: application to unfolded and native-like conformational fluctuations. *Chem. Phys.*, 307:217–225, 2004.
- [368] Benoit Roux and Klaus Schulten. Computational studies of membrane channels. *Structure*, 12:1343–1351, 2004.
- [369] Shigehiko Hayashi, Emad Tajkhorshid, Hideki Kandori, and Klaus Schulten. Role of hydrogen-bond network in energy storage of bacteriorhodopsin’s light-driven proton pump revealed by *ab initio* normal mode analysis. *J. Am. Chem. Soc.*, 126:10516–10517, 2004.
- [370] J. B. Heng, C. Ho, T. Kim, R. Timp, A. Aksimentiev, Y. V. Grinkova, S. Sligar, K. Schulten, and G. Timp. Sizing DNA using a nanometer-diameter pore. *Biophys. J.*, 87:2905–2911, 2004.

- [371] Aleksij Aksimentiev, Jiunn Benjamin Heng, Gregory Timp, and Klaus Schulten. Microscopic kinetics of DNA translocation through synthetic nanopores. *Biophys. J.*, 87:2086–2097, 2004.
- [372] Markus Dittrich, Shigehiko Hayashi, and Klaus Schulten. ATP hydrolysis in the β_{TP} and β_{DP} catalytic sites of F_1 -ATPase. *Biophys. J.*, 87:2954–2967, 2004.
- [373] Marcos Sotomayor and Klaus Schulten. Molecular dynamics study of gating in the mechanosensitive channel of small conductance MscS. *Biophys. J.*, 87:3050–3065, 2004.
- [374] David Craig, Mu Gao, Klaus Schulten, and Viola Vogel. Structural insights into how the MIDAS ion stabilizes integrin binding to an RGD peptide under force. *Structure*, 12:2049–2058, 2004.
- [375] Felix Autenrieth, Emad Tajkhorshid, Klaus Schulten, and Zaida Luthey-Schulten. Role of water in transient cytochrome c2 docking. *J. Phys. Chem. B*, 108:20376–20387, 2004.
- [376] Ioan Kosztin and Klaus Schulten. Fluctuation-driven molecular transport through an asymmetric membrane channel. *Phys. Rev. Lett.*, 93:238102, 2004. (4 pages).
- [377] Deyu Lu, Yan Li, Slava V. Rotkin, Umberto Ravaioli, and Klaus Schulten. Finite-size effect and wall polarization in a carbon nanotube channel. *Nano Lett.*, 4:2383–2387, 2004.
- [378] Fangqiang Zhu, Emad Tajkhorshid, and Klaus Schulten. Collective diffusion model for water permeation through microscopic channels. *Phys. Rev. Lett.*, 93:224501, 2004. (4 pages).
- [379] Jin Yu, Taekjip Ha, and Klaus Schulten. Conformational model of the Holliday junction transition deduced from molecular dynamics simulations. *Nucleic Acids Res.*, 32:6683–6695, 2004.
- [380] Amy Y. Shih, Iliia G. Denisov, James C. Phillips, Stephen G. Sligar, and Klaus Schulten. Molecular dynamics simulations of discoidal bilayers assembled from truncated human lipoproteins. *Biophys. J.*, 88:548–556, 2005.
- [381] Emad Tajkhorshid, Jordi Cohen, Aleksij Aksimentiev, Marcos Sotomayor, and Klaus Schulten. Towards understanding membrane channels. In Boris Martinac and Andrzej Kubalski, editors, *Bacterial ion channels and their eukaryotic homologues*, pp. 153–190. ASM Press, Washington, DC, 2005.
- [382] Melih Şener and Klaus Schulten. Physical principles of efficient excitation transfer in light harvesting. In David L. Andrews, editor, *Energy Harvesting Materials*, pp. 1–26. World Scientific, Singapore, 2005.
- [383] Yan Li, Deyu Lu, Slava V. Rotkin, Klaus Schulten, and Umberto Ravaioli. Screening of water dipoles inside finite-length armchair carbon nanotubes. *J. Comp. Electron.*, 4:161–165, 2005.
- [384] Emad Tajkhorshid, Fangqiang Zhu, and Klaus Schulten. Kinetic theory and simulation of single-channel water transport. In S. Yip, editor, *Handbook of Materials Modeling, Vol. I: Methods and Models*, pp. 1797–1822. Springer, Netherlands, 2005.
- [385] Jordi Cohen, Kwiseon Kim, Matthew Posewitz, Maria L. Ghirardi, Klaus Schulten, Michael Seibert, and Paul King. Molecular dynamics and experimental investigation of H_2 and O_2 diffusion in [Fe]-hydrogenase. *Biochem. Soc. Trans.*, 33:80–82, 2005.
- [386] Maria L. Ghirardi, Paul W. King, Matthew C. Posewitz, Pin Ching Maness, Alexander Fedorov, Kwiseon Kim, Jordi Cohen, Klaus Schulten, and Michael Seibert. Approaches to developing biological H_2 -photoproducing organisms and processes. *Biochem. Soc. Trans.*, 33:70–72, 2005.
- [387] Aleksij Aksimentiev and Klaus Schulten. Imaging alpha-hemolysin with molecular dynamics: Ionic conductance, osmotic permeability and the electrostatic potential map. *Biophys. J.*, 88:3745–3761, 2005.
- [388] Elizabeth Villa, Alexander Balaeff, and Klaus Schulten. Structural dynamics of the *Lac* repressor-DNA complex revealed by a multiscale simulation. *Proc. Natl. Acad. Sci. USA*, 102:6783–6788, 2005.

- [389] Marcos Sotomayor, David P. Corey, and Klaus Schulten. In search of the hair-cell gating spring: Elastic properties of ankyrin and cadherin repeats. *Structure*, 13:669–682, 2005.
- [390] Deyu Lu, Yan Li, Umberto Ravaioli, and Klaus Schulten. Empirical nanotube model for biological applications. *J. Phys. Chem. B*, 109:11461–11467, 2005.
- [391] J. B. Heng, A. Aksimentiev, C. Ho, P. Marks, Y. V. Grinkova, S. Sligar, K. Schulten, and G. Timp. Stretching DNA using an electric field in a synthetic nanopore. *Nano Lett.*, 5:1883–1888, 2005.
- [392] Yi Wang, Klaus Schulten, and Emad Tajkhorshid. What makes an aquaporin a glycerol channel: A comparative study of AqpZ and GlpF. *Structure*, 13:1107–1118, 2005.
- [393] Markus Dittrich, Peter L. Freddolino, and Klaus Schulten. When light falls in LOV: A quantum mechanical/molecular mechanical study of photoexcitation in Phot-LOV1 of *Chlamydomonas reinhardtii*. *J. Phys. Chem. B*, 109:13006–13013, 2005.
- [394] Jordi Cohen, Kwiseon Kim, Paul King, Michael Seibert, and Klaus Schulten. Finding gas diffusion pathways in proteins: Application to O₂ and H₂ transport in CpI [FeFe]-hydrogenase and the role of packing defects. *Structure*, 13:1321–1329, 2005.
- [395] J. B. Heng, A. Aksimentiev, C. Ho, V. Dimitrov, T. Sorsch, J. Miner, W. Mansfield, K. Schulten, and G. Timp. Beyond the gene chip. *Bell Labs Tech. J.*, 10:5–22, 2005.
- [396] Melih K. Sener, Craig Jolley, Adam Ben-Shem, Petra Fromme, Nathan Nelson, Roberta Croce, and Klaus Schulten. Comparison of the light harvesting networks of plant and cyanobacterial photosystem I. *Biophys. J.*, 89:1630–1642, 2005.
- [397] James Gumbart, Yi Wang, Aleksei Aksimentiev, Emad Tajkhorshid, and Klaus Schulten. Molecular dynamics simulations of proteins in lipid bilayers. *Curr. Opin. Struct. Biol.*, 15:423–431, 2005.
- [398] Jerome Mathé, Aleksei Aksimentiev, David R. Nelson, Klaus Schulten, and Amit Meller. Orientation discrimination of single stranded DNA inside the α -hemolysin membrane channel. *Proc. Natl. Acad. Sci. USA*, 102:12377–12382, 2005.
- [399] Laxmikant V. Kale, Klaus Schulten, Robert D. Skeel, Glenn Martyna, Mark Tuckerman, James C. Phillips, Sameer Kumar, and Gengbin Zheng. Biomolecular modeling using parallel supercomputers. In S. Aluru, editor, *Handbook of computational molecular biology*, pp. 34.1–34.43. Taylor and Francis, 2005.
- [400] James C. Phillips, Rosemary Braun, Wei Wang, James Gumbart, Emad Tajkhorshid, Elizabeth Villa, Christophe Chipot, Robert D. Skeel, Laxmikant Kale, and Klaus Schulten. Scalable molecular dynamics with NAMD. *J. Comp. Chem.*, 26:1781–1802, 2005.
- [401] Timothy A. Isgro and Klaus Schulten. Binding dynamics of isolated nucleoporin repeat regions to importin- β . *Structure*, 13:1869–1879, 2005.
- [402] Markus Dittrich and Klaus Schulten. Zooming in on ATP hydrolysis in F₁. *J. Bioenerg. Biomembr.*, 37:441–444, 2005.
- [403] Deyu Lu, Yan Li, Umberto Ravaioli, and Klaus Schulten. Ion-nanotube terahertz oscillator. *Phys. Rev. Lett.*, 95:246801, 2005. (4 pages).
- [404] J. B. Heng, A. Aksimentiev, C. Ho, P. Marks, Y. V. Grinkova, S. Sligar, K. Schulten, and G. Timp. The electromechanics of DNA in a synthetic nanopore. *Biophys. J.*, 90:1098–1106, 2006.
- [405] Amy Y. Shih, Anton Arkhipov, Peter L. Freddolino, and Klaus Schulten. Coarse grained protein-lipid model with application to lipoprotein particles. *J. Phys. Chem. B*, 110:3674–3684, 2006.

- [406] Peter L. Freddolino, Anton S. Arkhipov, Steven B. Larson, Alexander McPherson, and Klaus Schulten. Molecular dynamics simulations of the complete satellite tobacco mosaic virus. *Structure*, 14:437–449, 2006.
- [407] Maria E. Gracheva, Anlin Xiong, Aleksei Aksimentiev, Klaus Schulten, Gregory Timp, and Jean-Pierre Leburton. Simulation of the electric response of DNA translocation through a semiconductor nanopore-capacitor. *Nanotechnology*, 17:622–633, 2006.
- [408] Deyu Lu, Aleksei Aksimentiev, Amy Y. Shih, Eduardo Cruz-Chu, Peter L. Freddolino, Anton Arkhipov, and Klaus Schulten. The role of molecular modeling in bionanotechnology. *Phys. Biol.*, 3:S40–S53, 2006.
- [409] Eric H. Lee, Mu Gao, Nikos Pinotsis, Matthias Wilmanns, and Klaus Schulten. Mechanical strength of the titin Z1Z2/teletonin complex. *Structure*, 14:497–509, 2006.
- [410] James Gumbart and Klaus Schulten. Molecular dynamics studies of the archaeal translocon. *Biophys. J.*, 90:2356–2367, 2006.
- [411] Alexander Balaeff, L. Mahadevan, and Klaus Schulten. Modeling DNA loops using the theory of elasticity. *Phys. Rev. E*, 73:031919, 2006. (23 pages).
- [412] Mu Gao and Klaus Schulten. Onset of anthrax toxin pore formation. *Biophys. J.*, 90:3267–3279, 2006.
- [413] Marcos Sotomayor, Trudy A. van der Straaten, Umberto Ravaioli, and Klaus Schulten. Electrostatic properties of the mechanosensitive channel of small conductance MscS. *Biophys. J.*, 90:3496–3510, 2006.
- [414] Eduardo R. Cruz-Chu, Aleksei Aksimentiev, and Klaus Schulten. Water-silica force field for simulating nanodevices. *J. Phys. Chem. B*, 110:21497–21508, 2006.
- [415] Jordi Cohen, Anton Arkhipov, Rosemary Braun, and Klaus Schulten. Imaging the migration pathways for O₂, CO, NO, and Xe inside myoglobin. *Biophys. J.*, 91:1844–1857, 2006.
- [416] Grischa Raphael Meyer, Justin Gullingsrud, Klaus Schulten, and Boris Martinac. Molecular dynamics study of MscL interactions with a curved lipid bilayer. *Biophys. J.*, 91:1630–1637, 2006.
- [417] Anton Arkhipov, Peter L. Freddolino, Katsumi Imada, Keiichi Namba, and Klaus Schulten. Coarse-grained molecular dynamics simulations of a rotating bacterial flagellum. *Biophys. J.*, 91:4589–4597, 2006.
- [418] Markus Dittrich, Jin Yu, and Klaus Schulten. PcrA helicase, a molecular motor studied from the electronic to the functional level. *Topics in Current Chemistry*, 268:319–347, 2006.
- [419] Mu Gao, Marcos Sotomayor, Elizabeth Villa, Eric Lee, and Klaus Schulten. Molecular mechanisms of cellular mechanics. *Phys. Chem. Chem. Phys.*, 8:3692–3706, 2006.
- [420] Jin Yu, Taekjip Ha, and Klaus Schulten. Structure-based model of the stepping motor of PcrA helicase. *Biophys. J.*, 91:2097–2114, 2006.
- [421] Michael Hoffmann, Marius Wanko, Paul Strodel, Peter H. Koenig, Thomas Frauenheim, Klaus Schulten, Walter Thiel, Emad Tajkhorshid, and Marcus Elstner. Color tuning in rhodopsins: the mechanism for the spectral shift between bacteriorhodopsin and sensory rhodopsin II. *J. Am. Chem. Soc.*, 128:10808–10818, 2006.
- [422] Markus Dittrich and Klaus Schulten. PcrA helicase, a prototype ATP-driven molecular motor. *Structure*, 14:1345–1353, 2006.
- [423] Jerome Henin, Klaus Schulten, and Christophe Chipot. Conformational equilibrium in alanine-rich peptides probed by reversible stretching simulations. *J. Phys. Chem. B*, 110:16718–16723, 2006.

- [424] Fatemeh Khalili-Araghi, Emad Tajkhorshid, and Klaus Schulten. Dynamics of K^+ ion conduction through Kv1.2. *Biophys. J.*, 91:L72–L74, 2006.
- [425] Jin Yu, Andrea J. Yool, Klaus Schulten, and Emad Tajkhorshid. Mechanism of gating and ion conductivity of a possible tetrameric pore in Aquaporin-1. *Structure*, 14:1411–1423, 2006.
- [426] Peter L. Freddolino, Markus Dittrich, and Klaus Schulten. Dynamic switching mechanisms in LOV1 and LOV2 domains of plant phototropins. *Biophys. J.*, 91:3630–3639, 2006.
- [427] Maria L. Ghirardi, Jordi Cohen, Paul King, Klaus Schulten, Kwiseon Kim, and Michael Seibert. [FeFe]-hydrogenases and photobiological hydrogen production. In Lionel Vayssieres, editor, *Solar hydrogen and Nanotechnology*, volume 6340 of *Proc. SPIE*, pp. 253–258, 2006.
- [428] Paul W. King, Drazenka Svedruzic, Jordi Cohen, Klaus Schulten, Michael Seibert, and Maria L. Ghirardi. Structural and functional investigations of biological catalysts for optimization of solar-driven, H_2 production systems. In Lionel Vayssieres, editor, *Solar Hydrogen and Nanotechnology*, volume 6340 of *Proc. SPIE*, pp. 259–267, 2006.
- [429] Anton Arkhipov, Peter L. Freddolino, and Klaus Schulten. Stability and dynamics of virus capsids described by coarse-grained modeling. *Structure*, 14:1767–1777, 2006.
- [430] Eileen Puklin-Faucher, Mu Gao, Klaus Schulten, and Viola Vogel. How the headpiece hinge angle is opened: new insights into the dynamics of integrin activation. *J. Cell Biol.*, 175:349–360, 2006.
- [431] Ying Yin, Morten Ø. Jensen, Emad Tajkhorshid, and Klaus Schulten. Sugar binding and protein conformational changes in lactose permease. *Biophys. J.*, 91:3972–3985, 2006.
- [432] Sungchul Hohng, Ruobo Zhou, Michelle K. Nahas, Jin Yu, Klaus Schulten, David M. J. Lilley, and Taekjip Ha. Fluorescence-force spectroscopy maps two-dimensional reaction landscape of the Holliday junction. *Science*, 318:279–283, 2007.
- [433] Ioan Kosztin and Klaus Schulten. Molecular dynamics methods for bioelectronic systems in photosynthesis. In Thijs Aartsma and Joerg Matysik, editors, *Biophysical Techniques in Photosynthesis II*, volume 26 of *Advances in Photosynthesis and Respiration*, pp. 445–464. Springer, Dordrecht, 2008.
- [434] Andrew Aird, Jörg Wrachtrup, Klaus Schulten, and Carsten Tietz. Possible pathway for ubiquinone shuttling in *R. rubrum* revealed by molecular dynamics simulation. *Biophys. J.*, 92:23–33, 2007.
- [435] Hanning Chen, Boaz Ilan, Yujie Wu, Fangqiang Zhu, Klaus Schulten, and Gregory A. Voth. Charge delocalization in proton channels. I. The aquaporin channels and proton blockage. *Biophys. J.*, 92:46–60, 2007.
- [436] Yi Wang, Jordi Cohen, Walter F. Boron, Klaus Schulten, and Emad Tajkhorshid. Exploring gas permeability of cellular membranes and membrane channels with molecular dynamics. *J. Struct. Biol.*, 157:534–544, 2007.
- [437] Marcos Sotomayor, Valeria Vasquez, Eduardo Perozo, and Klaus Schulten. Ion conduction through MscS as determined by electrophysiology and simulation. *Biophys. J.*, 92:886–902, 2007.
- [438] Amy Y. Shih, Peter L. Freddolino, Anton Arkhipov, and Klaus Schulten. Assembly of lipoprotein particles revealed by coarse-grained molecular dynamics simulations. *J. Struct. Biol.*, 157:579–592, 2007.
- [439] Timothy A. Isgro and Klaus Schulten. Association of nuclear pore FG-repeat domains to NTF2 import and export complexes. *J. Mol. Biol.*, 366:330–345, 2007.
- [440] Ilia A. Solov'yov, Danielle E. Chandler, and Klaus Schulten. Magnetic field effects in Arabidopsis thaliana cryptochrome-1. *Biophys. J.*, 92:2711–2726, 2007.

- [441] Morten Ø. Jensen, Ying Yin, Emad Tajkhorshid, and Klaus Schulten. Sugar transport across lactose permease probed by steered molecular dynamics. *Biophys. J.*, 93:92–102, 2007.
- [442] Bryan J. Johnson, Jordi Cohen, Richard W. Welford, Arwen R. Pearson, Klaus Schulten, Judith P. Klinman, and Carrie M. Wilmot. Exploring molecular oxygen pathways in *Hanseluna Polymorpha* copper-containing amine oxidase. *J. Biol. Chem.*, 282:17767–17776, 2007.
- [443] Eric H. Lee, Jen Hsin, Olga Mayans, and Klaus Schulten. Secondary and tertiary structure elasticity of titin Z1Z2 and a titin chain model. *Biophys. J.*, 93:1719–1735, 2007.
- [444] Marcos Sotomayor and Klaus Schulten. Single-molecule experiments in vitro and in silico. *Science*, 316:1144–1148, 2007.
- [445] Amy Y. Shih, Peter L. Freddolino, Stephen G. Sligar, and Klaus Schulten. Disassembly of nanodiscs with cholate. *Nano Lett.*, 7:1692–1696, 2007.
- [446] Timothy A. Isgro and Klaus Schulten. Cse1p binding dynamics reveal a novel binding pattern for FG-repeat nucleoporins on transport receptors. *Structure*, 15:977–991, 2007.
- [447] Amy Y. Shih, Anton Arkhipov, Peter L. Freddolino, Stephen G. Sligar, and Klaus Schulten. Assembly of lipids and proteins into lipoprotein particles. *J. Phys. Chem. B*, 111:11095–11104, 2007.
- [448] Jin Yu, Taekjip Ha, and Klaus Schulten. How directional translocation is regulated in a DNA helicase motor. *Biophys. J.*, 93:3783–3797, 2007.
- [449] Jordi Cohen and Klaus Schulten. O₂ migration pathways are not conserved across proteins of a similar fold. *Biophys. J.*, 93:3591–3600, 2007.
- [450] James Gumbart and Klaus Schulten. Structural determinants of lateral gate opening in the protein translocon. *Biochemistry*, 46:11147–11157, 2007.
- [451] Shuxun Cui, Jin Yu, Ferdinand Kühner, Klaus Schulten, and Hermann E. Gaub. Double stranded DNA dissociates into single strands when dragged into a poor solvent. *J. Am. Chem. Soc.*, 129:14710–14716, 2007.
- [452] Anton Arkhipov, Jana Hüve, Martin Kahms, Reiner Peters, and Klaus Schulten. Continuous fluorescence microphotolysis and correlation spectroscopy using 4Pi microscopy. *Biophys. J.*, 93:4006–4017, 2007.
- [453] John E. Stone, James C. Phillips, Peter L. Freddolino, David J. Hardy, Leonardo G. Trabuco, and Klaus Schulten. Accelerating molecular modeling applications with graphics processors. *J. Comp. Chem.*, 28:2618–2640, 2007.
- [454] Francois Dehez, Janos G. Angyan, Ignacio Soteras Gutierrez, F. Javier Luque, Klaus Schulten, and Christophe Chipot. Modeling induction phenomena in intermolecular interactions with an ab initio force field. *J. Chem. Theory Comput.*, 3:1914–1926, 2007.
- [455] Melih K. Sener, John D. Olsen, C. Neil Hunter, and Klaus Schulten. Atomic level structural and functional model of a bacterial photosynthetic membrane vesicle. *Proc. Natl. Acad. Sci. USA*, 104:15723–15728, 2007.
- [456] Michelle Gower, Jordi Cohen, James Phillips, Richard Kufirin, and Klaus Schulten. Managing biomolecular simulations in a grid environment with NAMD-G. In *Proceedings of the 2006 TeraGrid Conference*, 2006. (7 pages).
- [457] Aleksei Aksimentiev, Robert Brunner, Jordi Cohen, Jeffrey Comer, Eduardo Cruz-Chu, David Hardy, Aruna Rajan, Amy Shih, Grigori Sigalov, Ying Yin, and Klaus Schulten. Computer modeling in biotechnology, a partner in development. In *Protocols in Nanostructure Design*, Methods in Molecular Biology, pp. 181–234. Humana Press, 2008.

- [458] Jerome Henin, Emad Tajkhorshid, Klaus Schulten, and Christophe Chipot. Diffusion of glycerol through *Escherichia coli* aquaglyceroporin GlpF. *Biophys. J.*, 94:832–839, 2008.
- [459] Klaus Schulten, James C. Phillips, Laxmikant V. Kalé, and Abhinav Bhatele. Biomolecular modeling in the era of petascale computing. In David Bader, editor, *Petascale Computing: Algorithms and Applications*, pp. 165–181. Chapman and Hall/CRC Press, Taylor and Francis Group, New York, 2008.
- [460] Jordi Cohen, Kenneth W. Olsen, and Klaus Schulten. Finding gas migration pathways in proteins using implicit ligand sampling. In Robert K. Poole, editor, *Globins and other NO-reactive Proteins in Microbes, Plants and Invertebrates*, volume 437 of *Methods in Enzymology*, pp. 437–455. Elsevier, 2008.
- [461] Peter L. Freddolino, Anton Arkhipov, Amy Y. Shih, Ying Yin, Zhongzhou Chen, and Klaus Schulten. Application of residue-based and shape-based coarse graining to biomolecular simulations. In Gregory A. Voth, editor, *Coarse-Graining of Condensed Phase and Biomolecular Systems*, chapter 20, pp. 299–315. Chapman and Hall/CRC Press, Taylor and Francis Group, 2008.
- [462] Amy Y. Shih, Peter L. Freddolino, Anton Arkhipov, Stephen G. Sligar, and Klaus Schulten. Molecular modeling of the structural properties and formation of high-density lipoprotein particles. In Scott Feller, editor, *Current Topics in Membranes: Computational Modeling of Membrane Bilayers*, chapter 11, pp. 313–342. Elsevier, 2008.
- [463] Valeria Vasquez, Marcos Sotomayor, D. Marien Cortes, Benoit Roux, Klaus Schulten, and Eduardo Perozo. Three dimensional architecture of membrane-embedded MscS in the closed conformation. *J. Mol. Biol.*, 378:55–70, 2008.
- [464] Christophe Chipot and Klaus Schulten. Understanding structure and function of membrane proteins using free energy calculations. In Eva Pebay-Peyroula, editor, *Biophysical analysis of membrane proteins. Investigating structure and function*, pp. 187–211. Wiley, Weinheim, 2008.
- [465] Bernard Lim, Eric H. Lee, Marcos Sotomayor, and Klaus Schulten. Molecular basis of fibrin clot elasticity. *Structure*, 16:449–459, 2008.
- [466] Aruna Rajan, Michael S. Strano, Daniel A. Heller, Tobias Hertel, and Klaus Schulten. Length dependent optical effects in single walled carbon nanotubes. *J. Phys. Chem. B*, 112:6211–6213, 2008.
- [467] Marcos Sotomayor and Klaus Schulten. The allosteric role of the Ca^{++} switch in adhesion and elasticity of C-cadherin. *Biophys. J.*, 94:4621–4633, 2008.
- [468] Christopher I. Rodrigues, David J. Hardy, John E. Stone, Klaus Schulten, and Wen-mei W. Hwu. GPU acceleration of cutoff pair potentials for molecular modeling applications. In *CF'08: Proceedings of the 2008 conference on Computing Frontiers*, pp. 273–282, New York, NY, USA, 2008. ACM.
- [469] Peter L. Freddolino, Feng Liu, Martin Gruebele, and Klaus Schulten. Ten-microsecond molecular dynamics simulation of a fast-folding WW domain. *Biophys. J.*, 94:L75–L77, 2008.
- [470] Basak Isin, Klaus Schulten, Emad Tajkhorshid, and Ivet Bahar. Mechanism of signal propagation upon retinal isomerization: Insights from molecular dynamics simulations of rhodopsin restrained by normal modes. *Biophys. J.*, 95:789–803, 2008.
- [471] Melih K. Şener and Klaus Schulten. From atomic-level structure to supramolecular organization in the photosynthetic unit of purple bacteria. In C. Neil Hunter, Fevzi Daldal, Marion C. Thurnauer, and J. Thomas Beatty, editors, *The Purple Phototrophic Bacteria*, volume 28 of *Advances in Photosynthesis and Respiration*, pp. 275–294. Springer, 2008.
- [472] Amy Y. Shih, Stephen G. Sligar, and Klaus Schulten. Molecular models need to be tested: the case of a solar flares discoidal HDL model. *Biophys. J.*, 94:L87–L89, 2008.

- [473] Leonardo G. Trabuco, Elizabeth Villa, Kakoli Mitra, Joachim Frank, and Klaus Schulten. Flexible fitting of atomic structures into electron microscopy maps using molecular dynamics. *Structure*, 16:673–683, 2008.
- [474] Zhongzhou Chen, Jizhong Lou, Cheng Zhu, and Klaus Schulten. Flow induced structural transition in the β -switch region of glycoprotein Ib. *Biophys. J.*, 95:1303–1313, 2008.
- [475] Ilia A. Solov'yov, Danielle Chandler, and Klaus Schulten. Exploring the possibilities for radical pair effects in cryptochrome. *Plant Signaling and Behavior*, 3:676–677, 2008.
- [476] James Gumbart and Klaus Schulten. The roles of pore ring and plug in the SecY protein-conducting channel. *J. Gen. Physiol.*, 132:709–719, 2008.
- [477] Danielle Chandler, Jen Hsin, Christopher B. Harrison, James Gumbart, and Klaus Schulten. Intrinsic curvature properties of photosynthetic proteins in chromatophores. *Biophys. J.*, 95:2822–2836, 2008.
- [478] Anton Arkhipov, Ying Yin, and Klaus Schulten. Four-scale description of membrane sculpting by BAR domains. *Biophys. J.*, 95:2806–2821, 2008.
- [479] Yongneng Yao, Christopher B. Harrison, Peter L. Freddolino, Klaus Schulten, and Mark L. Mayer. Molecular mechanisms of ligand recognition by NR3 subtype glutamate receptors. *EMBO J.*, 27:2158–2170, 2008.
- [480] Valeria Vasquez, Marcos Sotomayor, Julio Cordero-Morales, Klaus Schulten, and Eduardo Perozo. A structural mechanism for MscS gating in lipid bilayers. *Science*, 321:1210–1214, 2008.
- [481] James C. Phillips, John E. Stone, and Klaus Schulten. Adapting a message-driven parallel application to GPU-accelerated clusters. In *SC '08: Proceedings of the 2008 ACM/IEEE Conference on Supercomputing*, Piscataway, NJ, USA, 2008. IEEE Press. (9 pages).
- [482] Jen Hsin, Anton Arkhipov, Ying Yin, John E. Stone, and Klaus Schulten. Using VMD - an introductory tutorial. *Current Protocols - Bioinformatics*, 5:Unit 5.7, 2008. (48 pages).
- [483] Shigehiko Hayashi, Emad Tajkhorshid, and Klaus Schulten. Photochemical reaction dynamics of the primary event of vision studied by a hybrid molecular simulation. *Biophys. J.*, 96:403–416, 2009.
- [484] Utkur M. Mirsaidov, Winston Timp, Xueqing Zou, Valentin Dimitrov, Klaus Schulten, Andrew P. Feinberg, and Greg Timp. Nanoelectromechanics of methylated DNA in a synthetic nanopore. *Biophys. J.*, 96:L32–L34, 2009.
- [485] Eduardo R. Cruz-Chu, Aleksei Aksimentiev, and Klaus Schulten. Ionic current rectification through silica nanopores. *J. Phys. Chem. C*, 113:1850–1862, 2009.
- [486] David J. Hardy, John E. Stone, and Klaus Schulten. Multilevel summation of electrostatic potentials using graphics processing units. *J. Paral. Comp.*, 35:164–177, 2009.
- [487] Elizabeth Villa, Jayati Sengupta, Leonardo G. Trabuco, Jamie LeBarron, William T. Baxter, Tanvir R. Shaikh, Robert A. Grassucci, Poul Nissen, Måns Ehrenberg, Klaus Schulten, and Joachim Frank. Ribosome-induced changes in elongation factor Tu conformation control GTP hydrolysis. *Proc. Natl. Acad. Sci. USA*, 106:1063–1068, 2009.
- [488] Aleksei Aksimentiev, Robert K. Brunner, Eduardo Cruz-Chu, Jeffrey Comer, and Klaus Schulten. Modeling transport through synthetic nanopores. *IEEE Nanotech.*, 3:20–28, 2009.
- [489] Venkat Maruthamuthu, Klaus Schulten, and Deborah Leckband. Elasticity and rupture of a multi-domain neural cell adhesion molecule complex. *Biophys. J.*, 96:3005–3014, 2009.
- [490] Lingling Miao and Klaus Schulten. Transport-related structures and processes of the nuclear pore complex studied through molecular dynamics. *Structure*, 17:449–459, 2009.

- [491] Melih K. Sener, Jen Hsin, Leonardo G. Trabuco, Elizabeth Villa, Pu Qian, C. Neil Hunter, and Klaus Schulten. Structural model and excitonic properties of the dimeric RC-LH1-PufX complex from *Rhodobacter sphaeroides*. *Chem. Phys.*, 357:188–197, 2009.
- [492] John E. Stone, Jan Saam, David J. Hardy, Kirby L. Vandivort, Wen-mei W. Hwu, and Klaus Schulten. High performance computation and interactive display of molecular orbitals on GPUs and multi-core CPUs. In *Proceedings of the 2nd Workshop on General-Purpose Processing on Graphics Processing Units, ACM International Conference Proceeding Series*, volume 383, pp. 9–18, New York, NY, USA, 2009. ACM.
- [493] Anton Arkhipov and Klaus Schulten. Limits for reduction of effective focal volume in multiple-beam light microscopy. *Opt. Express*, 17:2861–2870, 2009.
- [494] Peter L. Freddolino, Sanghyun Park, Benoit Roux, and Klaus Schulten. Force field bias in protein folding simulations. *Biophys. J.*, 96:3772–3780, 2009.
- [495] Fatemeh Khalili-Araghi, James Gumbart, Po-Chao Wen, Marcos Sotomayor, Emad Tajkhorshid, and Klaus Schulten. Molecular dynamics simulations of membrane channels and transporters. *Curr. Opin. Struct. Biol.*, 19:128–137, 2009.
- [496] Ying Yin, Anton Arkhipov, and Klaus Schulten. Simulations of membrane tubulation by lattices of amphiphysin N-BAR domains. *Structure*, 17:882–892, 2009.
- [497] Iliia A. Solov'yov and Klaus Schulten. Magnetoreception through cryptochrome may involve superoxide. *Biophys. J.*, 96:4804–4813, 2009.
- [498] Leonardo G. Trabuco, Elizabeth Villa, Eduard Schreiner, Christopher B. Harrison, and Klaus Schulten. Molecular Dynamics Flexible Fitting: A practical guide to combine cryo-electron microscopy and X-ray crystallography. *Methods*, 49:174–180, 2009.
- [499] Jen Hsin, James Gumbart, Leonardo G. Trabuco, Elizabeth Villa, Pu Qian, C. Neil Hunter, and Klaus Schulten. Protein-induced membrane curvature investigated through molecular dynamics flexible fitting. *Biophys. J.*, 97:321–329, 2009.
- [500] Amy Y. Shih, Stephen G. Sligar, and Klaus Schulten. Maturation of high-density lipoproteins. *J. R. Soc. Interface*, 6:863–871, 2009.
- [501] Eduardo R. Cruz-Chu, Thorsten Ritz, Zuzanna S. Siwy, and Klaus Schulten. Molecular control of ionic conduction in polymer nanopores. *Faraday Discuss.*, 143:47–62, 2009.
- [502] James E. Knapp, Reinhard Pahl, Jordi Cohen, Jeffrey C. Nichols, Klaus Schulten, Quentin H. Gibson, Vukica Šrajcar, and William E. Royer Jr. Ligand migration and cavities within scapharca dimeric HbI: Studies by time-resolved crystallography, Xe binding, and computational analysis. *Structure*, 17:1494–1504, 2009.
- [503] Anton Arkhipov, Wouter H. Roos, Gijs J. L. Wuite, and Klaus Schulten. Elucidating the mechanism behind irreversible deformation of viral capsids. *Biophys. J.*, 97:2061–2069, 2009.
- [504] Peter L. Freddolino and Klaus Schulten. Common structural transitions in explicit-solvent simulations of villin headpiece folding. *Biophys. J.*, 97:2338–2347, 2009.
- [505] Anton Arkhipov, Ying Yin, and Klaus Schulten. Membrane-bending mechanism of amphiphysin N-BAR domains. *Biophys. J.*, 97:2727–2735, 2009.
- [506] Eric H. Lee, Jen Hsin, Marcos Sotomayor, Gemma Comellas, and Klaus Schulten. Discovery through the computational microscope. *Structure*, 17:1295–1306, 2009.

- [507] Danielle E. Chandler, James Gumbart, John D. Stack, Christophe Chipot, and Klaus Schulten. Membrane curvature induced by aggregates of LH2s and monomeric LH1s. *Biophys. J.*, 97:2978–2984, 2009.
- [508] Fabien Archambault, Christophe Chipot, Ignacio Soteras, F. Javier Luque, Klaus Schulten, and Francois Dehez. Polarizable intermolecular potentials for water and benzene interacting with halide and metal ions. *J. Chem. Theory Comput.*, 5:3022–3031, 2009.
- [509] James Gumbart, Leonardo G. Trabuco, Eduard Schreiner, Elizabeth Villa, and Klaus Schulten. Regulation of the protein-conducting channel by a bound ribosome. *Structure*, 17:1453–1464, 2009.
- [510] Thom H. Dunning Jr., Klaus Schulten, Jeroen Tromp, Jeremiah P. Ostriker, Kelvin Droegemeier, Ming Xue, and Paul Fussell. Science and engineering in the petascale era. *Comput. in Sci. and Eng.*, 11:28–36, 2009.
- [511] Jen Hsin, Chris Chipot, and Klaus Schulten. A glycophorin A-like framework for the dimerization of photosynthetic core complexes. *J. Am. Chem. Soc.*, 131:17096–17098, 2009.
- [512] Thomas Becker, Shashi Bhushan, Alexander Jarasch, Jean-Paul Armache, Soledad Funes, Fabrice Jossinet, James Gumbart, Thorsten Mielke, Otto Berninghausen, Klaus Schulten, Eric Westhof, Reid Gilmore, Elisabet C. Mandon, and Roland Beckmann. Structure of monomeric yeast and mammalian Sec61 complexes interacting with the translating ribosome. *Science*, 326:1369–1373, 2009.
- [513] Birgit Seidelt, C. Axel Innis, Daniel N. Wilson, Marco Gartmann, Jean-Paul Armache, Elizabeth Villa, Leonardo G. Trabuco, Thomas Becker, Thorsten Mielke, Klaus Schulten, Thomas A. Steitz, and Roland Beckmann. Structural insight into nascent polypeptide chain-mediated translational stalling. *Science*, 326:1412–1415, 2009.
- [514] Johan Strümpfer and Klaus Schulten. Light harvesting complex II B850 excitation dynamics. *J. Chem. Phys.*, 131:225101, 2009. (9 pages).
- [515] Ly Le, Eric H. Lee, Klaus Schulten, and Thahn Truong. Molecular modeling of swine influenza A/H1N1, Spanish H1N1, and avian H5N1 flu N1 neuraminidases bound to Tamiflu and Relenza. *PLoS Currents: Influenza*, 2009 Aug 27:RRN1015, 2010. (9 pages).
- [516] Eric H. Lee, Jen Hsin, Eleonore von Castelmuur, Olga Mayans, and Klaus Schulten. Tertiary and secondary structure elasticity of a six-Ig titin chain. *Biophys. J.*, 98:1085–1095, 2010.
- [517] Ying Yin, Anton Arkhipov, and Klaus Schulten. Multi-scale simulations of membrane sculpting by N-BAR domains. In Philip Biggin and Mark Sansom, editors, *Molecular Simulations and Biomembranes: From Biophysics to Function*, chapter 6, pp. 146–176. Royal Society of Chemistry, 2010.
- [518] Lingling Miao and Klaus Schulten. Probing a structural model of the nuclear pore complex channel through molecular dynamics. *Biophys. J.*, 98:1658–1667, 2010.
- [519] Jen Hsin, Danielle E. Chandler, James Gumbart, Christopher B. Harrison, Melih Sener, Johan Strumpfer, and Klaus Schulten. Self-assembly of photosynthetic membranes. *ChemPhysChem*, 11:1154–1159, 2010.
- [520] Leonardo G. Trabuco, Christopher B Harrison, Eduard Schreiner, and Klaus Schulten. Recognition of the regulatory nascent chain TnaC by the ribosome. *Structure*, 18:627–637, 2010.
- [521] Fatemeh Khalili-Araghi, Vishwanath Jogini, Vladimir Yarov-Yarovoy, Emad Tajkhorshid, Benoit Roux, and Klaus Schulten. Calculation of the gating charge for the Kv1.2 voltage-activated potassium channel. *Biophys. J.*, 98:2189–2198, 2010.
- [522] Aruna Rajan, Peter L. Freddolino, and Klaus Schulten. Going beyond clustering in MD trajectory analysis: an application to villin headpiece folding. *PLoS One*, 5:e9890, 2010. (12 pages).

- [523] Ilia A. Solov'yov, Henrik Mouritsen, and Klaus Schulten. Acuity of a cryptochrome and vision based magnetoreception system in birds. *Biophys. J.*, 99:40–49, 2010.
- [524] Melih Sener, Johan Strumpfer, John A. Timney, Arvi Freiberg, C. Neil Hunter, and Klaus Schulten. Photosynthetic vesicle architecture and constraints on efficient energy harvesting. *Biophys. J.*, 99:67–75, 2010.
- [525] Ilia A. Solov'yov, Klaus Schulten, and Walter Greiner. How birds and other animals orient in the Earth magnetic field. *Physik Journal*, 9:23–28, 2010. (article in German only).
- [526] Ly Le, Eric H. Lee, David J. Hardy, Thanh N. Truong, and Klaus Schulten. Molecular dynamics simulations suggest that electrostatic funnel directs binding of Tamiflu to influenza N1 neuraminidases. *PLoS Comput. Biol.*, 6:e1000939, 2010. (13 pages).
- [527] Peter L. Freddolino, Christopher B. Harrison, Yanxin Liu, and Klaus Schulten. Challenges in protein folding simulations. *Nature Phys.*, 6:751–758, 2010.
- [528] Xueqing Zou, Yanxin Liu, Zhongzhou Chen, Gloria Ines Cárdenas-Jirón, and Klaus Schulten. Flow-induced β -hairpin folding of the glycoprotein Iba β -switch. *Biophys. J.*, 99:1182–1191, 2010.
- [529] Wouter H. Roos, Melissa M. Gibbons, Anton Arkhipov, Charlotte Uetrecht, Norman Watts, Paul Wingfield, Alasdair C. Steven, Albert J.R.Heck, Klaus Schulten, William S. Klug, and Gijs J.L. Wuite. Squeezing protein shells: how continuum elastic models, molecular dynamics simulations and experiments coalesce at the nanoscale. *Biophys. J.*, 99:1175–1181, 2010.
- [530] Jan Saam, Elena Rosini, Gianluca Molla, Klaus Schulten, Loredano Pollegioni, and Sandro Ghisla. O₂-reactivity of flavoproteins: Dynamic access of dioxygen to the active site and role of a H⁺ relay system in D-amino acid oxidase. *J. Biol. Chem.*, 285:24439–24446, 2010.
- [531] Jen Hsin, Johan Strümpfer, Melih Sener, Pu Qian, C. Neil Hunter, and Klaus Schulten. Energy transfer dynamics in an RC-LH1-PufX tubular photosynthetic membrane. *New J. Phys.*, 12:085005, 2010. (19 pages).
- [532] Eduardo R. Cruz-Chu and Klaus Schulten. Computational microscopy of the role of protonable surface residues in nanoprecipitation oscillations. *ACS Nano*, 4:4463–4474, 2010.
- [533] John E. Stone, David J. Hardy, Ivan S. Ufimtsev, and Klaus Schulten. GPU-accelerated molecular modeling coming of age. *J. Mol. Graph. Model.*, 29:116–125, 2010.
- [534] Aleksandra Kijac, Amy Y. Shih, Andrew J. Nieuwkoop, Klaus Schulten, Stephen G. Sligar, and Chad Rienstra. Lipid-protein correlations in nanoscale phospholipid bilayers determined by solid-state nuclear magnetic resonance. *Biochemistry*, 49:9190–9198, 2010.
- [535] HyeongJun Kim, Jen Hsin, Yanxin Liu, Paul R. Selvin, and Klaus Schulten. Formation of salt bridges mediates internal dimerization of myosin VI medial tail domain. *Structure*, 18:1443–1449, 2010.
- [536] Leonardo G. Trabuco, Eduard Schreiner, John Eargle, Peter Cornish, Taekjip Ha, Zaida Luthey-Schulten, and Klaus Schulten. The role of L1 stalk-tRNA interaction in the ribosome elongation cycle. *J. Mol. Biol.*, 402:741–760, 2010.
- [537] John E. Stone, Axel Kohlmeyer, Kirby L. Vandivort, and Klaus Schulten. Immersive molecular visualization and interactive modeling with commodity hardware. *Lect. Notes in Comp. Sci.*, 6454:382–393, 2010.
- [538] John E. Stone, David J. Hardy, Barry Isralewitz, and Klaus Schulten. GPU algorithms for molecular modeling. In Jack Dongarra, David A. Bader, and Jakub Kurzak, editors, *Scientific Computing with Multicore and Accelerators*, chapter 16, pp. 351–371. Chapman & Hall/CRC Press, 2011.

- [539] John E. Stone, David J. Hardy, Jan Saam, Kirby L. Vandivort, and Klaus Schulten. GPU-accelerated computation and interactive display of molecular orbitals. In Wen-mei Hwu, editor, *GPU Computing Gems*, chapter 1, pp. 5–18. Morgan Kaufmann Publishers, 2011.
- [540] David J. Hardy, John E. Stone, Kirby L. Vandivort, David Gohara, Christopher Rodrigues, and Klaus Schulten. Fast molecular electrostatics algorithms on GPUs. In Wen-mei Hwu, editor, *GPU Computing Gems*, chapter 4, pp. 43–58. Morgan Kaufmann Publishers, 2011.
- [541] Leonardo G. Trabuco, Eduard Schreiner, James Gumbart, Jen Hsin, Elizabeth Villa, and Klaus Schulten. Applications of the molecular dynamics flexible fitting method. *J. Struct. Biol.*, 173:420–427, 2011.
- [542] Carsten Olbrich, Johan Strümpfer, Klaus Schulten, and Ulrich Kleinekathoefer. Quest for spatially correlated fluctuations in the FMO light-harvesting complex. *J. Phys. Chem. B*, 115:758–764, 2011.
- [543] James Gumbart, Eduard Schreiner, Leonardo G. Trabuco, Kwok-Yan Chan, and Klaus Schulten. Viewing the mechanisms of translation through the computational microscope. In Joachim Frank, editor, *Molecular Machines in Biology*, chapter 8, pp. 142–157. Cambridge University Press, 2011.
- [544] Johan Strümpfer, Jen Hsin, Melih Sener, Danielle Chandler, and Klaus Schulten. The light-harvesting apparatus in purple photosynthetic bacteria, introduction to a quantum biological device. In Benoit Roux, editor, *Molecular Machines*, chapter 2, pp. 19–48. World Scientific Press, 2011.
- [545] Jen Hsin, Johan Strümpfer, Eric H. Lee, and Klaus Schulten. Molecular origin of the hierarchical elasticity of titin: simulation, experiment and theory. *Annu. Rev. Biophys.*, 40:187–203, 2011.
- [546] Wen Li, Leonardo G. Trabuco, Klaus Schulten, and Joachim Frank. Molecular dynamics of EF-G during translocation. *Proteins: Struct., Func., Bioinf.*, 79:1478–1486, 2011.
- [547] Wei Jiang, David Hardy, James Phillips, Alex MacKerell, Klaus Schulten, and Benoit Roux. High-performance scalable molecular dynamics simulations of a polarizable force field based on classical Drude oscillators in NAMD. *J. Phys. Chem. Lett.*, 2:87–92, 2011.
- [548] Wei Chen, Jizhong Lou, Jen Hsin, Klaus Schulten, Stephen C. Harvey, and Cheng Zhu. Molecular dynamics simulations of forced unbending of integrin $\alpha_V\beta_3$. *PLoS Comput. Biol.*, 7(2):e1001086, 2011. (13 pages).
- [549] Melih Sener, Johan Strümpfer, Jen Hsin, Danielle Chandler, Simon Scheuring, C. Neil Hunter, and Klaus Schulten. Förster energy transfer theory as reflected in the structures of photosynthetic light harvesting systems. *ChemPhysChem*, 12:518–531, 2011.
- [550] James Gumbart, Christophe Chipot, and Klaus Schulten. Free-energy cost for translocon-assisted insertion of membrane proteins. *Proc. Natl. Acad. Sci. USA*, 108:3596–3601, 2011.
- [551] Jen Hsin and Klaus Schulten. Improved resolution of tertiary structure elasticity in muscle protein. *Biophys. J.*, 100:L22–L24, 2011.
- [552] Gregory Timp, Utkur Mirsaidov, Winston Timp, Jiwook Shim, Deqiang Wang, Valentin Dimitrov, Jan Scrimgeour, Chunchen Lin, Jeffrey Comer, Anthony Ho, Xueqing Zou, Aleksei Aksimentiev, and Klaus Schulten. 3rd generation DNA sequencing with a nanopore. In Samir M. Iqbal and Rashid Bashir, editors, *Nanopores: Sensing and Fundamental Biological Interactions*, chapter 12, pp. 287–312. Springer, Berlin, 2011.
- [553] Jens Frauenfeld, James Gumbart, Eli O. van der Sluis, Soledad Funes, Marco Gartmann, Birgitta Beatrix, Thorsten Mielke, Otto Berninghausen, Thomas Becker, Klaus Schulten, and Roland Beckmann. Cryo-EM structure of the ribosome-SecYE complex in the membrane environment. *Nat. Struct. Mol. Biol.*, 18:614–621, 2011.

- [554] Xabier Agirrezabala, Eduard Schreiner, Leonardo G. Trabuco, Jianlin Lei, Rodrigo F. Ortiz-Meoz, Klaus Schulten, Rachel Green, and Joachim Frank. Structural insights into cognate vs. near-cognate discrimination during decoding. *EMBO J.*, 30:1497–1507, 2011.
- [555] Yi Wang, Chris B. Harrison, Klaus Schulten, and J. Andrew McCammon. Implementation of accelerated molecular dynamics in NAMD. *Comput. Sci. Discov.*, 4:015002, 2011. (11 pages).
- [556] Johan Strümpfer and Klaus Schulten. The effect of correlated bath fluctuations on exciton transfer. *J. Chem. Phys.*, 134:095102, 2011. (9 pages).
- [557] David E. Tanner, Kwok-Yan Chan, James Phillips, and Klaus Schulten. Parallel generalized Born implicit solvent calculations with NAMD. *J. Chem. Theory Comput.*, 7:3635–3642, 2011.
- [558] Chaitanya Sathe, Xueqing Zou, Jean-Pierre Leburton, and Klaus Schulten. Computational investigation of DNA detection using graphene nanopores. *ACS Nano*, 5:8842–8851, 2011.
- [559] Sang-Hun Song, Peter Freddolino, Abigail Nash, Elizabeth Carroll, Klaus Schulten, Kevin Gardner, and Delmar S. Larsen. Modulating LOV domain photodynamics with a residue alteration outside the chromophore binding site. *Biochemistry*, 50:2411–2423, 2011.
- [560] Ulrich Kleinekathoefer, Barry Isralewitz, Markus Dittrich, and Klaus Schulten. Domain motion of individual F₁-ATPase β -subunits during unbiased molecular dynamics simulations. *J. Phys. Chem.*, 115:7267–7274, 2011.
- [561] James Gumbart, Christophe Chipot, and Klaus Schulten. Free energy of nascent-chain folding in the translocon. *J. Am. Chem. Soc.*, 133:7602–7607, 2011.
- [562] David E. Tanner, Wen Ma, Zhongzhou Chen, and Klaus Schulten. Theoretical and computational investigation of flagellin translocation and bacterial flagellum growth. *Biophys. J.*, 100:2548–2556, 2011.
- [563] Yanxin Liu, Jen Hsin, HyeongJun Kim, Paul R Selvin, and Klaus Schulten. Extension of a three-helix bundle domain of myosin VI and key role of calmodulins. *Biophys. J.*, 100:2964–2973, 2011.
- [564] Eduard Schreiner, Leonardo G. Trabuco, Peter L. Freddolino, and Klaus Schulten. Stereochemical errors and their implications for molecular dynamics simulations. *BMC Bioinform.*, 12:190, 2011. (9 pages).
- [565] Ramya Gamini, Marcos Sotomayor, Christophe Chipot, and Klaus Schulten. Cytoplasmic domain filter function in the mechanosensitive channel of small conductance. *Biophys. J.*, 101:80–89, 2011.
- [566] Carsten Olbrich, Thomas L. C. Jansen, Jörg Liebers, Mortaza Aghtar, Johan Strümpfer, Klaus Schulten, Jasper Knoester, and Ulrich Kleinekathoefer. From atomistic modeling to excitation transfer and two-dimensional spectra of the FMO light-harvesting complex. *J. Phys. Chem. B*, 115(26):8609–8621, 2011.
- [567] Philip M.D. Severin, Xueqing Zou, Hermann E. Gaub, and Klaus Schulten. Cytosine methylation alters DNA mechanical properties. *Nucleic Acids Res.*, 39:8740–8751, 2011.
- [568] John E. Stone, Kirby L. Vandivort, and Klaus Schulten. Immersive out-of-core visualization of large-size and long-timescale molecular dynamics trajectories. *Lect. Notes in Comp. Sci.*, 6939:1–12, 2011.
- [569] Carsten Olbrich, Johan Strümpfer, Klaus Schulten, and Ulrich Kleinekathoefer. Theory and simulation of the environmental effects on FMO electronic transitions. *J. Phys. Chem. Lett.*, 2:1771–1776, 2011.
- [570] Jen Hsin, Loren LaPointe, Alla Kazy, Christophe Chipot, Alessandro Senes, and Klaus Schulten. Oligomerization state of photosynthetic core complexes is correlated with the dimerization affinity of a transmembrane helix. *J. Am. Chem. Soc.*, 133:14071–14081, 2011.

- [571] Kwok-Yan Chan, James Gumbart, Ryan McGreevy, Jean M. Watermeyer, B. Trevor Sewell, and Klaus Schulten. Symmetry-restrained flexible fitting for symmetric EM maps. *Structure*, 19:1211–1218, 2011.
- [572] Wei Han and Klaus Schulten. Further optimization of a hybrid united-atom and coarse-grained force field for folding simulations: Improved backbone hydration and interactions between charged side chains. *J. Chem. Theory Comput.*, 8:4413–4424, 2012.
- [573] Ernesto Vargas, Vladimir Yarov-Yarovoy, Fatemeh Khalili-Araghi, William A. Catterall, Michael L. Klein, Mounir Tarek, Erik Lindahl, Klaus Schulten, Eduardo Perozo, Francisco Bezanilla, and Benot Roux. Viewpoint: An emerging consensus on voltage-dependent gating from computational modeling and molecular dynamics simulations. *J. Gen. Physiol.*, 140:587–594, 2012.
- [574] Xueqing Zou, Wen Ma, Ilia Solov'yov, Christophe Chipot, and Klaus Schulten. Recognition of methylated DNA through methyl-CpG binding domain proteins. *Nucleic Acids Res.*, 40:2747–2758, 2012.
- [575] Fatemeh Khalili-Araghi, Emad Tajkhorshid, Benoit Roux, and Klaus Schulten. Molecular dynamics investigation of the ω current in the Kv1.2 voltage sensor domains. *Biophys. J.*, 102:258–267, 2012.
- [576] Johan Strumpfer, Melih Sener, and Klaus Schulten. How quantum coherence assists photosynthetic light harvesting. *J. Phys. Chem. Lett.*, 3:536–542, 2012.
- [577] Ilia A. Solov'yov and Klaus Schulten. Reaction kinetics and mechanism of magnetic field effects in cryptochrome. *J. Phys. Chem. B*, 116:1089–1099, 2012.
- [578] Xabier Agirrezabala, Hstau Liao, Eduard Schreiner, Jie Fu, Rodrigo Ortiz-Meoz, Klaus Schulten, Rachel Green, and Joachim Frank. Structural characterization of mRNA-tRNA translocation intermediates. *Proc. Natl. Acad. Sci. USA*, 109:6094–6099, 2012.
- [579] Kwok-Yan Chan, Leonardo G. Trabuco, Eduard Schreiner, and Klaus Schulten. Cryo-electron microscopy modeling by the molecular dynamics flexible fitting method. *Biopolymers*, 97:678–686, 2012.
- [580] Michael Krone, John E. Stone, Thomas Ertl, and Klaus Schulten. Fast visualization of Gaussian density surfaces for molecular dynamics and particle system trajectories. In *EuroVis - Short Papers 2012*, pp. 67–71, 2012.
- [581] Yanxin Liu, Johan Strümpfer, Peter L. Freddolino, Martin Gruebele, and Klaus Schulten. Structural characterization of λ -repressor folding from all-atom molecular dynamics simulations. *J. Phys. Chem. Lett.*, 3:1117–1123, 2012.
- [582] Whasil Lee, Johan Strümpfer, Vann Bennett, Klaus Schulten, and Piotr E. Marszalek. Mutation of conserved histidines alters the tertiary structure and nanomechanics of consensus ankyrin repeats. *J. Biol. Chem.*, 287:19115–19121, 2012.
- [583] Mortaza Aghtar, Jörg Liebers, Johan Strümpfer, Klaus Schulten, and Ulrich Kleinekathöfer. Juxtaposing density matrix and classical path-based wave packet dynamics. *J. Chem. Phys.*, 136:214101, 2012. (9 pages).
- [584] Christopher Harrison and Klaus Schulten. Quantum and classical dynamics simulations of ATP hydrolysis in solution. *J. Chem. Theory Comput.*, 8:2328–2335, 2012.
- [585] James Gumbart, Eduard Schreiner, Daniel N. Wilson, Roland Beckmann, and Klaus Schulten. Mechanisms of SecM-mediated stalling in the ribosome. *Biophys. J.*, 103:331–341, 2012.
- [586] Martin van Eijk, Michael J. Rynkiewicz, Mitchell R. White, Kevan L. Hartshorn, Xueqing Zou, Klaus Schulten, Dong Luo, Erika C. Crouch, Tanya M. Cafarella, James F. Head, Henk P. Haagsman, and Barbara A. Seaton. Unique sugar-binding site mediates the distinct anti-influenza activity of pig surfactant protein D. *J. Biol. Chem.*, 287:26666–26677, 2012.

- [587] Johan Strümpfer and Klaus Schulten. Open quantum dynamics calculations with the hierarchy equations of motion on parallel computers. *J. Chem. Theory Comput.*, 8:2808–2816, 2012.
- [588] David E. Tanner, James C. Phillips, and Klaus Schulten. GPU/CPU algorithm for generalized Born / solvent-accessible surface area implicit solvent calculations. *J. Chem. Theory Comput.*, 8:2521–2530, 2012.
- [589] Eleonore von Castelmur, Johan Strümpfer, Barbara Franke, Julijus Bogomolovas, Sonia Barbieri, Hiroshi Qadota, Petr V. Konarev, Dmitri I. Svergun, Siegfried Labeit, Guy M. Benian, Klaus Schulten, and Olga Mayans. Identification of an N-terminal inhibitory extension as the primary mechanosensory regulator of twitchin kinase. *Proc. Natl. Acad. Sci. USA*, 109:13608–13613, 2012.
- [590] Johan Strümpfer and Klaus Schulten. Excited state dynamics in photosynthetic reaction center and light harvesting complex 1. *J. Chem. Phys.*, 137:065101, 2012. (8 pages).
- [591] Ilia A. Solov'yov, Po-Yao Chang, and Klaus Schulten. Vibrationally assisted electron transfer mechanism of olfaction: Myth or reality? *Phys. Chem. Chem. Phys.*, 14:13861–13871, 2012.
- [592] Danielle E. Chandler, Francois Penin, Klaus Schulten, and Christophe Chipot. The p7 protein of hepatitis C virus forms structurally plastic, minimalist ion channels. *PLoS Comput. Biol.*, 8:e1002702, 2012. (10 pages).
- [593] Yi Chen, Eduardo R. Cruz-Chu, Jaie Woodard, Manas Ranjan Gartia, Klaus Schulten, and Logan Liu. Electrically induced conformational change of peptides on metallic nano-surfaces. *ACS Nano*, 6:8847–8856, 2012.
- [594] Ariela Vergara-Jaque, Horacio Poblete, Eric Lee, Klaus Schulten, Fernando González-Nilo, and Christophe Chipot. Molecular basis of drug resistance in A/H1N1 virus. *J. Chem. Inf. Model.*, 52:2650–2656, 2012.
- [595] Ilia A. Solov'yov, Tatiana Domratcheva, Abdul R. M. Shahi, and Klaus Schulten. Decrypting cryptochrome: Revealing the molecular identity of the photoactivation reaction. *J. Am. Chem. Soc.*, 134:18046–18052, 2012.
- [596] John E. Stone, Barry Isralewitz, and Klaus Schulten. Early experiences scaling VMD molecular visualization and analysis jobs on Blue Waters. In *Extreme Scaling Workshop (XSW), 2013*, pp. 43–50, Aug. 2013.
- [597] John E. Stone, Kirby L. Vandivort, and Klaus Schulten. GPU-accelerated molecular visualization on petascale supercomputing platforms. In *Proceedings of the 8th International Workshop on Ultrascale Visualization*, UltraVis '13, pp. 6:1–6:8, New York, NY, USA, 2013. ACM.
- [598] Boon Chong Goh, Michael J. Rynkiewicz, Tanya R. Cafarella, Mitchell R. White, Kevan L. Hartshorn, Kimberly Allen, Erika C. Crouch, Oliviana Calin, Peter H. Seeberger, Klaus Schulten, and Barbara A. Seaton. Molecular mechanisms of inhibition of influenza by surfactant protein D revealed by large-scale molecular dynamics simulation. *Biochemistry*, 52:8527–8538, 2013.
- [599] Philip M.D. Severin, Xueqing Zou, Klaus Schulten, and Hermann E. Gaub. Effects of cytosine hydroxymethylation on DNA strand separation. *Biophys. J.*, 104:208–215, 2013.
- [600] Xue Wang, Fengting Xu, Jiasen Liu, Bingquan Gao, Yanxin Liu, Yujia Zhai, Jun Ma, Kai Zhang, Timothy S. Baker, Klaus Schulten, Dong Zheng, Hai Pang, and Fei Sun. Atomic model of rabbit hemorrhagic disease virus by cryo-electron microscopy and crystallography. *PLoS Pathog.*, 9:e1003132, 2013. (14 pages).
- [601] Hang Yu and Klaus Schulten. Membrane sculpting by F-BAR domains studied by molecular dynamics simulations. *PLoS Comput. Biol.*, 9:e1002892, 2013. (15 pages).

- [602] Markita P. Landry, Xueqing Zou, Lei Wang, Wai Mun Huang, Klaus Schulten, and Yann R. Chemla. DNA target sequence identification mechanism for dimer-active protein complexes. *Nucleic Acids Res.*, 41:2416–2427, 2013.
- [603] Ying Lai, Jiajie Diao, Yanxin Liu, Yuji Ishitsuka, Zengliu Su, Klaus Schulten, Taekjip Ha, and Yeon-Kyun Shin. Fusion pore formation and expansion induced by Ca^{2+} and synaptotagmin 1. *Proc. Natl. Acad. Sci. USA*, 110:1333–1338, 2013.
- [604] James C. Gumbart, Ivan Teo, Benoit Roux, and Klaus Schulten. Reconciling the roles of kinetic and thermodynamic factors in membrane-protein insertion. *J. Am. Chem. Soc.*, 135:2291–2297, 2013.
- [605] Wen Li, Gemma C. Atkinson, Nehal S. Thakor, Ülar Allas, Chuao-chao Lu, Kwok-Yan Chan, Tanel Tenson, Klaus Schulten, Kevin S. Wilson, Vasili Hauryliuk, and Joachim Frank. Mechanism of tetracycline resistance by ribosomal protection protein Tet(O). 4:1477, 2013. (8 pages).
- [606] Jiwook Shim, Gwendolyn I. Humphreys, Bala Murali Venkatesan, Jan Marie Munz, Xueqing Zou, Chaitanya Sathe, Klaus Schulten, Farhad Kosari, Ann M. Nardulli, George Vasmatzis, and Rashid Bashir. Detection and quantification of methylation in DNA using solid-state nanopores. *Sci. Rep.*, 3:1389, 2013. (8 pages).
- [607] Peter L. Freddolino, Kevin H. Gardner, and Klaus Schulten. Signaling mechanisms of LOV domains: new insights from molecular dynamics studies. *Photochem. Photobiol. Sci.*, 12:1158–1170, 2013.
- [608] Maxim B. Prigozhin, Yanxin Liu, Anna Jean Wirth, Shobhna Kapoor, Roland Winter, Klaus Schulten, and Martin Gruebele. Misplaced helix slows down ultrafast pressure-jump protein folding. *Proc. Natl. Acad. Sci. USA*, 110:8087–8092, 2013.
- [609] Antony R. Crofts, Sangjin Hong, Charles Wilson, Rodney Burton, Doreen Victoria, Chris Harrison, and Klaus Schulten. The mechanism of ubihydroquinone oxidation at the Q_o -site of the cytochrome bc_1 complex. *Biochim. Biophys. Acta*, 1827:1362–1377, 2013.
- [610] Kai Zhang, Li Wang, Yanxin Liu, Kwok-Yan Chan, Xiaoyun Pang, Klaus Schulten, Zhiyang Dong, and Fei Sun. Flexible interwoven termini determine the thermal stability of thermosomes. *Protein & Cell*, 4:432–444, 2013.
- [611] Mortaza Aghtar, Johan Strümpfer, Carsten Olbrich, Klaus Schulten, and Ulrich Kleinekathoefer. The FMO complex in a glycerol-water mixture. *J. Phys. Chem. B*, 117:7157–7163, 2013.
- [612] Gongpu Zhao, Juan R. Perilla, Ernest L. Yufenyuy, Xin Meng, Bo Chen, Jiying Ning, Jinwoo Ahn, Angela M. Gronenborn, Klaus Schulten, Christopher Aiken, and Peijun Zhang. Mature HIV-1 capsid structure by cryo-electron microscopy and all-atom molecular dynamics. *Nature*, 497:643–646, 2013.
- [613] Christopher G. Mayne, Jan Saam, Klaus Schulten, Emad Tajkhorshid, and James C. Gumbart. Rapid parameterization of small molecules using the Force Field Toolkit. *J. Comp. Chem.*, 34:2757–2770, 2013.
- [614] Wei Han and Klaus Schulten. Characterization of folding mechanisms of Trp-cage and WW-domain by network analysis of simulations with a hybrid-resolution model. *J. Phys. Chem. B*, 117:13367–13377, 2013.
- [615] Ivan Teo and Klaus Schulten. A computational kinetic model of diffusion for molecular systems. *J. Chem. Phys.*, 139:121929, 2013. (15 pages).
- [616] Anuj Girdhar, Chaitanya Sathe, Klaus Schulten, and Jean-Pierre Leburton. Graphene quantum point contact transistor for DNA sensing. *Proc. Natl. Acad. Sci. USA*, 110:16748–16753, 2013.
- [617] Wei Jiang, James Phillips, Lei Huang, Mikolai Fajer, Yilin Meng, James Gumbart, Yun Luo, Klaus Schulten, and Benoit Roux. Generalized scalable multiple copy algorithms for molecular dynamics simulations in NAMD. *Comput. Phys. Commun.*, 185:908–916, 2014.

- [618] Iliia Solov'yov, Tatiana Domratcheva, and Klaus Schulten. Separation of photo-induced radical pair in cryptochrome to a functionally critical distance. *Sci. Rep.*, 4:3845, 2014. (8 pages).
- [619] Ioan Kosztin and Klaus Schulten. Structure, function, and quantum dynamics of pigment-protein complexes. In Masoud Mohseni, Yasser Omar, Greg Engel, and Martin B. Plenio, editors, *Quantum Effects in Biology*, pp. 123–143. Cambridge University Press, 2014.
- [620] Iliia A. Solov'yov, P. J. Hore, Thorsten Ritz, and Klaus Schulten. A chemical compass for bird navigation. In Masoud Mohseni, Yasser Omar, Greg Engel, and Martin B. Plenio, editors, *Quantum Effects in Biology*, chapter 10, pp. 218–236. Cambridge University Press, 2014.
- [621] Shigehiko Hayashi and Klaus Schulten. Quantum biology of retinal. In Masoud Mohseni, Yasser Omar, Greg Engel, and Martin B. Plenio, editors, *Quantum Effects in Biology*, pp. 237–263. Cambridge University Press, 2014.
- [622] Qufei Li, Sherry Wanderling, Marcin Paduch, David Medovoy, Abhishek Singharoy, Ryan McGreevy, Carlos Villalba-Galea, Raymond E. Hulse, Benoit Roux, Klaus Schulten, Anthony Kossiakoff, and Eduardo Perozo. Structural mechanism of voltage-dependent gating in an isolated voltage-sensing domain. *Nat. Struct. Mol. Biol.*, 21:244–252, 2014.
- [623] Ramya Gamini, Wei Han, John E. Stone, and Klaus Schulten. Assembly of Nsp1 nucleoporins provides insight into nuclear pore complex gating. *PLoS Comput. Biol.*, 10:e1003488, 2014. (14 pages).
- [624] Yong Wang, Yanxin Liu, Hannah A. DeBerg, Takeshi Nomura, Melinda Tonks Hoffman, Paul R. Rohde, Klaus Schulten, Boris Martinac, and Paul R. Selvin. Single molecule FRET reveals pore size and opening mechanism of MscL. *eLife*, 3:e01834, 2014. (21 pages).
- [625] Yanxin Liu, Maxim B. Prigozhin, Klaus Schulten, and Martin Gruebele. Observation of complete pressure-jump protein refolding in molecular dynamics simulation and experiment. *J. Am. Chem. Soc.*, 136:4265–4272, 2014.
- [626] Jeffrey Comer, Klaus Schulten, and Christophe Chipot. Calculation of lipid-bilayer permeabilities using an average force. *J. Chem. Theory Comput.*, 10:554–564, 2014.
- [627] Michaël L. Cartron, John D. Olsen, Melih Sener, Philip J. Jackson, Amanda A. Brindley, Pu Qian, Mark J. Dickman, Graham J. Leggett, Klaus Schulten, and C. Neil Hunter. Integration of energy and electron transfer processes in the photosynthetic membrane of *Rhodobacter sphaeroides*. *Biochim. Biophys. Acta – Bioener.*, 1837:1769–1780, 2014.
- [628] Qiangjun Zhou, Jiangmei Li, Hang Yu, Yujia Zhai, Zhen Gao, Yanxin Liu, Xiaoyun Pang, Lunfeng Zhang, Klaus Schulten, Fei Sun, and Chang Chen. Molecular insights into the membrane-associated phosphatidylinositol 4-kinase II α . *Nat. Commun.*, 5:3552, 2014. (10 pages).
- [629] Yifei Qi, Xi Cheng, Wei Han, Sunhwan Jo, Klaus Schulten, and Wonpil Im. CHARMM-GUI PACE CG builder for solution, micelle, and bilayer coarse-grained simulations. *J. Chem. Inf. Model.*, 54:1003–1009, 2014.
- [630] John E. Stone, Ryan McGreevy, Barry Isralewitz, and Klaus Schulten. GPU-accelerated analysis and visualization of large structures solved by molecular dynamics flexible fitting. *Faraday Discuss.*, 169:265–283, 2014.
- [631] Danielle Chandler, Johan Strümpfer, Melih Sener, Simon Scheuring, and Klaus Schulten. Light harvesting by lamellar chromatophores in *Rhodospirillum photometricum*. *Biophys. J.*, 106:2503–2510, 2014.
- [632] Lela Vukovic, Hye Ran Koh, Sua Myong, and Klaus Schulten. Substrate recognition and specificity of double-stranded RNA binding proteins. *Biochemistry*, 53:3457–3466, 2014.

- [633] Jeffrey Comer, Klaus Schulten, and Christophe Chipot. Diffusive models of membrane permeation with explicit orientational freedom. *J. Chem. Theory Comput.*, 10:2710–2718, 2014.
- [634] Rafael C. Bernardi, Isaac Cann, and Klaus Schulten. Molecular dynamics study of enhanced Man5B enzymatic activity. *Biotechnol. Biofuels*, 7:1–8, 2014.
- [635] Shanmugapriya Sothiselvam, Bo Liu, Wei Han, Dorota Klepacki, Gemma C. Atkinson, Age Brauer, Maido Remm, Tanel Tenson, Klaus Schulten, Nora Vázquez-Laslop, and Alexander S. Mankin. Macrolide antibiotics allosterically predispose the ribosome for translation arrest. *Proc. Natl. Acad. Sci. USA*, 111:9804–9809, 2014.
- [636] Ryan McGreevy, Abhishek Singharoy, Qufei Li, Jingfen Zhang, Dong Xu, Eduardo Perozo, and Klaus Schulten. xMDFF: Molecular dynamics flexible fitting of low-resolution X-Ray structures. *Acta Cryst. D*, 70:2344–2355, 2014.
- [637] Anuj Girdhar, Chaitanya Sathe, Klaus Schulten, and Jean-Pierre Leburton. Gate-modulated graphene quantum point contact device for DNA sensing. *J. Comp. Electron.*, 13:839–846, 2014.
- [638] Stephan Wickles, Abhishek Singharoy, Jessica Andreani, Stefan Seemayer, Lukas Bischoff, Otto Berninghausen, Johannes Soeding, Klaus Schulten, Eli van der Sluis, and Roland Beckmann. A structural model of the active ribosome-bound membrane protein insertase YidC. *eLife*, 3:e03035, 2014. (17 pages).
- [639] Zhe Wu and Klaus Schulten. Synaptotagmin’s role in neurotransmitter release likely involves Ca^{2+} -induced conformational transition. *Biophys. J.*, 107:1156–1166, 2014.
- [640] En Cai, Pinghua Ge, Sang Hak Lee, Okunola Jeyifous, Yong Wang, Yanxin Liu, Katie Wilson, Sung Jun Lim, Michelle Baird, John Stone, Kwan Young Lee, Michael Davidson, Hee Jung Chung, Klaus Schulten, Andrew Smith, William Green, and Paul R. Selvin. Stable small quantum dots for synaptic receptor tracking on live neurons. *Angew. Chem. Int. Ed. Engl.*, 126:12692–12696, 2014.
- [641] Wei Han and Klaus Schulten. Fibril elongation by $\text{A}\beta_{17-42}$: Kinetic network analysis of hybrid-resolution molecular dynamics simulations. *J. Am. Chem. Soc.*, 136:12450–12460, 2014.
- [642] Mortaza Aghtar, Johann Strümpfer, Carsten Olbrich, Klaus Schulten, and Ulrich Kleinekathoefer. On the different types of vibrations interacting with electronic excitations in the PE545 and FMO antenna systems. *J. Phys. Chem. Lett.*, 5:3131–3137, 2014.
- [643] Andrew E. Blanchard, Mark J. Arcario, Klaus Schulten, and Emad Tajkhorshid. A highly tilted membrane configuration for the pre-fusion state of synaptobrevin. *Biophys. J.*, 107:2112–2121, 2014.
- [644] Chaitanya Sathe, Anuj Girdhar, Jean-Pierre Leburton, and Klaus Schulten. Electronic detection of dsDNA transition from helical to zipper conformation using graphene nanopores. *Nanotechnology*, 25:445105, 2014. (9 pages).
- [645] Melih Sener, John E. Stone, Angela Barragan, Abhishek Singharoy, Ivan Teo, Kirby L. Vandivort, Barry Isralewitz, Bo Liu, Boon Chong Goh, James C. Phillips, Lena F. Kourkoutis, C. Neil Hunter, and Klaus Schulten. Visualization of energy conversion processes in a light harvesting organelle at atomic detail. In *Proceedings of the International Conference on High Performance Computing, Networking, Storage and Analysis*, SC ’14. IEEE Press, 2014. (4 pages).
- [646] James C. Phillips, John E. Stone, Kirby L. Vandivort, Timothy G. Armstrong, Justin M. Wozniak, Michael Wilde, and Klaus Schulten. Petascale Tcl with NAMD, VMD, and Swift/T. In *SC’14 workshop on High Performance Technical Computing in Dynamic Languages*, SC ’14, pp. 6–17. IEEE Press, 2014.
- [647] Constantin Schoeler, Klara H. Malinowska, Rafael C. Bernardi, Lukas F. Milles, Markus A. Jobst, Ellis Durner, Wolfgang Ott, Daniel B. Fried, Edward A. Bayer, Klaus Schulten, Hermann E. Gaub, and Michael A. Nash. Ultrastable cellulosome-adhesion complex tightens under load. *Nat. Commun.*, 5:5635, 2014.

- [648] Till Rudack, Juan Perilla, and Klaus Schulten. Die Geheimnisse des Lebens berechnen. *Spektrum Wiss.*, 11:86–95, November 2014.
- [649] Jeffrey Comer, James Phillips, Klaus Schulten, and Christophe Chipot. Multiple-replica strategies for free-energy calculations in NAMD: Multiple-walker adaptive biasing force and walker selection rules. *J. Chem. Theory Comput.*, 10:5276–5285, 2014.
- [650] Milana Fraiberg, Oshri Afanзар, C. Keith Cassidy, Alexandra Gabashvili, Klaus Schulten, Yishai Levin, and Michael Eisenbach. CheY’s acetylation sites responsible for generating clockwise flagellar rotation in *Escherichia coli*. *Mol. Microbiol.*, 95:231–244, 2015.
- [651] Angela M. Barragan, Antony R. Crofts, Klaus Schulten, and Ilia A. Solov’yov. Identification of ubiquinol binding motifs at the Q_o-site of the cytochrome bc₁ complex. *J. Phys. Chem. B*, 119:433–447, 2015.
- [652] David J. Hardy, Zhe Wu, James C. Phillips, John E. Stone, Robert D. Skeel, and Klaus Schulten. Multilevel summation method for electrostatic force evaluation. *J. Chem. Theory Comput.*, 11:766–779, 2015.
- [653] Rafael C. Bernardi, Marcelo C. R. Melo, and Klaus Schulten. Enhanced sampling techniques in molecular dynamics simulations of biological systems. *Biochim. Biophys. Acta*, 1850:872–877, 2015.
- [654] Wen Ma and Klaus Schulten. Mechanism of substrate translocation by a ring-shaped ATPase motor at millisecond resolution. *J. Am. Chem. Soc.*, 137:3031–3040, 2015.
- [655] Anuj Girdhar, Chaitanya Sathe, Klaus Schulten, and Jean-Pierre Leburton. Tunable graphene quantum point contact transistor for DNA detection and characterization. *Nanotechnology*, 26:134005, 2015. (10 pages).
- [656] Juan R. Perilla, Boon Chong Goh, C. Keith Cassidy, Bo Liu, Rafael C. Bernardi, Till Rudack, Hang Yu, Zhe Wu, and Klaus Schulten. Molecular dynamics simulations of large macromolecular complexes. *Curr. Opin. Struct. Biol.*, 31:64–74, 2015.
- [657] Michael T. Englander, Joshua L. Avins, Rachel C. Fleisher, Bo Liu, Philip R. Efraim, Jiangning Wang, Klaus Schulten, Thomas S. Leyh, Ruben L. Gonzalez Jr., and Virginia W. Cornish. The ribosome can discriminate the chirality of amino acids within its peptidyl-transferase center. *Proc. Natl. Acad. Sci. USA*, 112:6038–6043, 2015.
- [658] Markita P. Landry, Lela Vukovic, Sebastian Kruss, Gili Bisker, Alexandra M. Landry, Shahrin Islam, Rishabh Jain, Klaus Schulten, and Michael S. Strano. Comparative dynamics and sequence dependence of DNA and RNA binding to single walled carbon nanotubes. *J. Phys. Chem. C*, 119:10048–10058, 2015.
- [659] Anna Jean Wirth, Yanxin Liu, Maxim B. Prigozhin, Klaus Schulten, and Martin Gruebele. Comparing fast pressure jump and temperature jump protein folding experiments and simulations. *J. Am. Chem. Soc.*, 137:7152–7159, 2015.
- [660] Boon Chong Goh, Juan R. Perilla, Matthew R. England, Katrina J. Heyrana, Rebecca C. Craven, and Klaus Schulten. Atomic modeling of an immature retroviral lattice using molecular dynamics and mutagenesis. *Structure*, 23:1414–1425, 2015.
- [661] Abhishek Singharoy, Balasubramanian Venkatakrishnan, Yun Liu, Christopher G. Mayne, Chun-Hsing Chen, Adam Zlotnick, Klaus Schulten, and Amar H. Flood. Macromolecular crystallography for synthetic abiological molecules: Combining xMDFE and PHENIX for structure determination of cyanostar macrocycles. *J. Am. Chem. Soc.*, 137:8810–8818, 2015.
- [662] Xinlei Wang, Lela Vukovic, Hye Ran Koh, Klaus Schulten, and Sua Myong. Dynamic profiling of double-stranded RNA binding proteins. *Nucleic Acids Res.*, 43:7566–7576, 2015.

- [663] Constantin Schoeler, Rafael C. Bernardi, Klara H. Malinowska, Ellis Durner, Wolfgang Ott, Edward A. Bayer, Klaus Schulten, Michael A. Nash, and Hermann E. Gaub. Mapping mechanical force propagation through biomolecular complexes. *Nano Lett.*, 15:7370–7376, 2015.
- [664] Santosh K. Misra, Goutam Ghoshal, Manas R. Gartia, Zhe Wu, Mao Ye, Corinne R. Bromfield, Emery M. Williams, Krishnarao V. Tangella, Klaus Schulten, Partha S. Ray, Everette C. Burdette, and Dipanjan Pan. Tri-Modal therapy: Combining hyperthermia with repurposed bexarotene and ultrasound for treating liver cancer. *ACS Nano*, 9:10695–10718, 2015.
- [665] Rong Shen, Wei Han, Giacomo Fiorin, Shahidul M. Islam, Klaus Schulten, and Benoit Roux. Structural refinement of proteins by restrained molecular dynamics simulations with non-interacting molecular fragments. *PLoS Comput. Biol.*, 11:e1004368, 2015. (19 pages).
- [666] Juan R. Perilla, Boon Chong Goh, John Stone, and Klaus Schulten. Chemical visualization of human pathogens: the Retroviral Capsids. *Proceedings of the 2015 ACM/IEEE Conference on Supercomputing*, 2015. (4 pages).
- [667] Manman Lu, Guangjin Hou, Huilan Zhang, Christopher L. Suiter, Jinwoo Ahn, In-Ja L. Byeon, Juan R. Perilla, Christopher J. Langmead, Ivan Hung, Peter L. Gor'kov, Zhehong Gan, William Brey, Christopher Aiken, Peijun Zhang, Klaus Schulten, Angela M. Gronenborn, and Tatyana Polenova. Dynamic allostery governs cyclophilin A-HIV capsid interplay. *Proc. Natl. Acad. Sci. USA*, 112:14617–14622, 2015.
- [668] Pulkit Gupta, Bo Liu, Dorota Klepacki, Vrinda Gupta, Klaus Schulten, Alexander S. Mankin, and Nora Vazquez-Laslop. Nascent peptide assists the ribosome in recognizing chemically distinct small molecules. *Nat. Chem. Biol.*, pp. (6 pages), 2015. PMID: 26727240.
- [669] Hang Yu, Wei Han, Wen Ma, and Klaus Schulten. Transient β -hairpin formation in α -synuclein monomer revealed by coarse-grained molecular dynamics simulation. *J. Chem. Phys.*, 143:243142, 2015.
- [670] C. Keith Cassidy, Benjamin A. Himes, Frances J. Alvarez, Jun Ma, Gongpu Zhao, Juan R. Perilla, Klaus Schulten, and Peijun Zhang. CryoEM and computer simulations reveal a novel kinase conformational switch in bacterial chemotaxis signaling. *eLife*, 10.7554/eLife.08419, 2015. PMID: 26583751.
- [671] Hu Qiu, Aditya Sarathy, Jean-Pierre Leburton, and Klaus Schulten. Intrinsic stepwise translocation of stretched ssDNA in graphene nanopores. *Nano Lett.*, 15:8322–8330, 2015.
- [672] John E. Stone, Melih Sener, Kirby L. Vandivort, Angela Barragan, Abhishek Singharoy, Ivan Teo, Joao V. Ribeiro, Barry Isralewitz, Bo Liu, Boon Chong Goh, James C. Phillips, Craig MacGregor-Chatwin, Matthew P. Johnson, Lena F. Kourkoutis, C. Neil Hunter, and Klaus Schulten. Atomic detail visualization of photosynthetic membranes with GPU-accelerated ray tracing. *Parallel Computing*, 55:17–27, 2016.
- [673] Ryan McGreevy, Ivan Teo, Abhishek Singharoy, and Klaus Schulten. Advances in the molecular dynamics flexible fitting method for cryo-EM modeling. *Methods*, 100:50–60, 2016.
- [674] Boon Chong Goh, Jodi A. Hadden, Rafael C. Bernardi, Abhishek Singharoy, Ryan McGreevy, Till Rudack, C. Keith Cassidy, and Klaus Schulten. Computational methodologies for real-space structural refinement of large macromolecular complexes. *Annu. Rev. Biophys.*, 45:253–278, 2016.
- [675] Lela Vukovic, Christophe Chipot, Debora L. Makino, Elena Conti, and Klaus Schulten. Molecular mechanism of processive 3' to 5' RNA translocation in the active subunit of the RNA exosome complex. *J. Am. Chem. Soc.*, 138:4069–4078, 2016.

- [676] Chuang Liu, Juan R. Perilla, Jiying Ning, Manman Lu, Guangjin Hou, Ruben Ramalho, Gregory Bedwell, In-Ja Byeon, Jinwoo Ahn, Jiong Shi, Angela Gronenborn, Peter Prevelige, Itay Rouso, Christopher Aiken, Tatyana Polenova, Klaus Schulten, and Peijun Zhang. Cyclophilin A stabilizes HIV-1 capsid through a novel non-canonical binding site. *Nat. Commun.*, 7:10714:(10 pages), 2016.
- [677] David J. Hardy, Matthew A. Wolff, Jianlin Xia, Klaus Schulten, and Robert D. Skeel. Multilevel summation with B-spline interpolation for pairwise interactions in molecular dynamics simulations. *J. Chem. Phys.*, 144:114112, 2016. (16 pages).
- [678] John E. Stone, William R. Sherman, and Klaus Schulten. Immersive molecular visualization with omnidirectional stereoscopic ray tracing and remote rendering. *2016 IEEE International Parallel and Distributed Processing Symposium Workshop (IPDPSW)*, pp. 1048–1057, 2016.
- [679] John E. Stone, Peter Messmer, Robert Sisneros, and Klaus Schulten. High performance molecular visualization: In-situ and parallel rendering with EGL. *2016 IEEE International Parallel and Distributed Processing Symposium Workshop (IPDPSW)*, pp. 1014–1023, 2016.
- [680] John E. Stone, Michael J. Hallock, James C. Phillips, Joseph R. Peterson, Zaida Luthey-Schulten, and Klaus Schulten. Evaluation of emerging energy-efficient heterogeneous computing platforms for biomolecular and cellular simulation workloads. *2016 IEEE International Parallel and Distributed Processing Symposium Workshop (IPDPSW)*, pp. 89–100, 2016.
- [681] Hu Qiu, Anuj Girdhar, Klaus Schulten, and Jean-Pierre Leburton. Electrically tunable quenching of DNA fluctuations in biased solid-state nanopores. *ACS Nano*, 10:4482–4488, 2016.
- [682] Yi Zhang, Klaus Schulten, Martin Gruebele, Paramjit S. Bansal, David Wilson, and Norelle L. Daly. Disulfide bridges: bringing together frustrated structure in a bioactive peptide. *Biophys. J.*, 110:1744–1752, 2016.
- [683] Yi Zhang, Lela Vukovic, Till Rudack, Wei Han, and Klaus Schulten. Recognition of poly-ubiquitins by the proteasome through protein re-folding guided by electrostatic and hydrophobic interactions. *J. Phys. Chem. B*, 120:8137–8146, 2016.
- [684] Yun Liu, Abhishek Singharoy, Christopher G. Mayne, Arkajyoti Sengupta, Krishnan Raghavachari, Klaus Schulten, and Amar H. Flood. Flexibility coexists with shape persistence in cyanostar macrocycles. *J. Am. Chem. Soc.*, 138:4843–4851, 2016.
- [685] Katrina Heyrana, Boon Chong Goh, Juan Roberto Perilla, Tam-Linh N. Nguyen, Matthew R. England, Maria C. Bewley, Klaus Schulten, and Rebecca Craven. Contributions of charged residues in structurally dynamic capsid surface loops to Rous sarcoma virus assembly. *J. Virol.*, 90:5700–5714, 2016.
- [686] Juan R. Perilla, Jodi A. Hadden, Boon Chong Goh, Christopher G. Mayne, and Klaus Schulten. All-atom molecular dynamics of virus capsids as drug targets. *J. Phys. Chem. Lett.*, 7:1836–1844, 2016.
- [687] Joao V. Ribeiro, Rafael C. Bernardi, Till Rudack, John E. Stone, James C. Phillips, Peter L. Freddolino, and Klaus Schulten. QwikMD-integrative molecular dynamics toolkit for novices and experts. *Sci. Rep.*, 6:26536, 2016.
- [688] Ivan Teo, Christopher G. Mayne, Klaus Schulten, and Tony Lelievre. Adaptive multilevel splitting method for molecular dynamics calculation of benzamidine-trypsin dissociation time. *J. Chem. Theory Comput.*, 12:2983–2989, 2016.
- [689] Jihong Tong, Zhe Wu, Margaret M. Briggs, Klaus Schulten, and Thomas J. McIntosh. The water permeability and pore entrance structure of aquaporin-4 channels depend on lipid bilayer thickness. *Biophys. J.*, 111:90–99, 2016.

- [690] John E. Stone, Antti-Pekka Hynninen, James C. Phillips, and Klaus Schulten. Early experiences porting the NAMD and VMD molecular simulation and analysis software to GPU-accelerated OpenPOWER platforms. *International Workshop on OpenPOWER for HPC (IWOPH'16)*, pp. 188–206, 2016.
- [691] Boon Chong Goh, Huixing Wu, Michael J. Rynkiewicz, Klaus Schulten, Barbara A. Seaton, and Francis X. McCormack. Elucidation of lipid binding sites on lung surfactant protein A using X-ray crystallography, mutagenesis and molecular dynamics simulations. *Biochemistry*, 55:3692–3701, 2016.
- [692] Kumud R Poudel, Yongming Dong, Hang Yu, Allen Su, Thuong Ho, Yan Liu, Klaus Schulten, and Jihong Bai. A time-course of orchestrated endophilin action in sensing, bending, and stabilizing curved membranes. *Mol. Biol. Cell*, 27:2119–2132, 2016.
- [693] Julian Deeng, Kwok-Yan Chan, Eli O. van der Sluis, Lukas Bischoff, Otto Berninghausen, Wei Han, James Gumbart, Klaus Schulten, Birgitta Beatrix, and Roland Beckmann. Dynamic behavior of trigger factor on the ribosome. *J. Mol. Biol.*, 428:3588–3602, 2016.
- [694] Andreas Schweitzer, Antje Aufderheide, Till Rudack, Florian Beck, Gunter Pfeifer, Jurgen M. Plitzko, Eri Sakata, Klaus Schulten, Friedrich Förster, and Wolfgang Baumeister. The structure of the human 26S proteasome at a resolution of 3.9 Å. *Proc. Natl. Acad. Sci. USA*, 113:7816–7821, 2016.
- [695] Abhishek Singharoy, Ivan Teo, Ryan McGreevy, John E. Stone, Jianhua Zhao, and Klaus Schulten. Molecular dynamics-based refinement and validation for sub-5 Å cryo-electron microscopy maps. *eLife*, 10.7554/eLife.16105, 2016. (66 pages).
- [696] Melih Sener, Johan Strümpfer, Abhishek Singharoy, C. Neil Hunter, and Klaus Schulten. Overall energy conversion efficiency of a photosynthetic vesicle. *eLife*, 10.7554/eLife.09541, 2016. (30 pages).
- [697] Aaron T. Bozzi, Lukas B. Bane, Wilhelm Weihofen, Anne McCabe, Abhishek Singharoy, Chris Chipot, Klaus Schulten, and Rachelle Gaudet. Conserved methionine dictates substrate preference in Nramp-family divalent metal transporters. *Proc. Natl. Acad. Sci. USA*, 113:10310–10315, 2016.
- [698] Abhishek Singharoy, Angela M. Barragan, Sundarapandian Thangapandian, Emad Tajkhorshid, and Klaus Schulten. Binding site recognition and docking dynamics of a single electron transport protein: Cytochrome c_2 . *J. Am. Chem. Soc.*, 138:12077–12089, 2016.
- [699] David F. Thieker, Jodi A. Hadden, Klaus Schulten, and Robert J. Woods. 3D implementation of the symbol nomenclature for graphical representation of glycans. *Glycobiology*, 26:786–787, 2016.
- [700] Angela M. Barragan, Klaus Schulten, and Ilia A. Solov'yov. Mechanism of the primary charge transfer reaction in the cytochrome bc1 complex. *J. Phys. Chem. B*, 120:11369–11380, 2016.
- [701] Aaron T. Bozzi, Lukas B. Bane, Wilhelm A. Weihofen, Abhishek Singharoy, Eduardo R. Guillen, Hidde L. Ploegh, Klaus Schulten, and Rachelle Gaudet. Crystal structure and conformational change mechanism of a bacterial Nramp-family divalent metal transporter. *Structure*, 24:2102–2114, 2016.
- [702] Huilan Zhang, Guangjin Hou, Manman Lu, Jinwoo Ahn, In-Ja L. Byeon, Christopher J. Langmead, Juan R. Perilla, Ivan Hung, Peter L. Gor'kov, Zhehong Gan, William W. Brey, David A. Case, Klaus Schulten, Angela M. Gronenborn, and Tatyana Polenova. HIV-1 capsid function is regulated by dynamics: Quantitative atomic-resolution insights by integrating magic-angle-spinning NMR, QM/MM, and MD. *J. Am. Chem. Soc.*, 138:14066–14075, 2016.
- [703] Mathieu Botte, Nathan Zaccai, Jelger Lycklama à Nijeholt, Remy Martin, Kèvin Knoops, Gabor Papai, Juan Zou, Aurélien Deniaud, Manikandan Karuppasamy, Qiyang Jiang, Abhishek Singha Roy, Klaus Schulten, Patrick Schultz, Juri Rappsilber, Giuseppe Zaccai, Imre Berger, Ian Collinson, and Christiane Schaffitzel. A central cavity within the holo-translocon suggests a mechanism for membrane protein insertion. *Sci. Rep.*, 6:38399, 2016.

- [704] Abhishek Singharoy, Christophe Chipot, Mahmoud Moradi, and Klaus Schulten. Chemomechanical coupling in hexameric protein-protein interfaces harnesses energy within V-type ATPases. *J. Am. Chem. Soc.*, 139:293–310, 2016.
- [705] Yifei Qi, Jumin Lee, Abhishek Singharoy, Ryan McGreevy, Klaus Schulten, and Wonpil Im. CHRMM-GUI MDFF/xMDFF utilizer for molecular dynamics flexible fitting simulations in various environments. *J. Phys. Chem. B*, 121:3718–3723, 2016.
- [706] Marc Wehmer, Till Rudack, Florian Beck, Antje Aufderheide, Günter Pfeifer, Jürgen M. Plitzko, Friedrich Förster, Klaus Schulten, Wolfgang Baumeister, and Eri Sakata. Structural insights into the functional cycle of the ATPase module of the 26S proteasome. *Proc. Natl. Acad. Sci. USA*, 114:1305–1310, 2017.
- [707] Suvrajit Maji, Rezvan Shahoei, Klaus Schulten, and Joachim Frank. Quantitative characterization of domain motions in molecular machines. *J. Phys. Chem. B*, 121:3747–3756, 2017.
- [708] Hu Qiu, Aditya Sarathy, Klaus Schulten, and Jean-Pierre Leburton. Detection and mapping of DNA methylation with 2D material nanopores. *npj 2D Mater. App.*, 1:3, 2017.
- [709] Venkata Giridhar Poosarla, Tong Li, Boon Chong Goh, Klaus Schulten, Thomas K. Wood, and Costas D. Maranas. Computational de novo design of antibodies binding to a peptide with high affinity. *Biotechnol. Bioeng.*, 114:1331–1342, 2017.
- [710] Lisa G. Lippert, Tali Dadosh, Jodi A. Hadden, Benjamin T. Diroll, Christopher B. Murray, Erika L.F. Holzbaur, Klaus Schulten, Samara L. Reck-Peterson, and Yale E. Goldman. Angular measurements of the dynein ring reveal a stepping mechanism dependent on a flexible stalk. *Proc. Natl. Acad. Sci. USA*, 114:E4564–E4573, 2017.
- [711] Jonne Seppälä, Rafael C. Bernardi, Tatu J. K. Haataja, Maarit Hellman, Olli T. Pentikäinen, Klaus Schulten, Perttu Permi, Jari Yläne, and Ulla Pentikäinen. Skeletal dysplasia mutations effect on human filamins’ structure and mechanosensing. *Sci. Rep.*, 7:4218, 2017.
- [712] Juan R. Perilla and Klaus Schulten. Physical properties of the HIV-1 capsid from all-atom molecular dynamics simulations. *Nat. Commun.*, 8:15959, 2017.
- [713] Jeffrey Comer, Klaus Schulten, and Christophe Chipot. Permeability of a fluid lipid bilayer to short-chain alcohols from first principles. *J. Chem. Theory Comput.*, 13:2523–2532, 2017.
- [714] Jiwook Shim, Shouvik Banerjee, Hu Qiu, Kirby K. H. Smithe, David Estrada, Julian Bello, Eric Pop, Klaus Schulten, and Rashid Bashir. Detection of methylation on dsDNA using nanopores in a MoS₂ membrane. *Nanoscale*, 9:14836–14845, 2017.
- [715] Frances J. D. Alvarez, Shaoda He, Juan R. Perilla, Sooin Jang, Klaus Schulten, Alan N. Engelman, Sjors H. W. Scheres, and Peijun Zhang. CryoEM structure of MxB reveals a novel oligomerization interface critical for HIV restriction. *Science Advances*, 3:e1701264, 2017.
- [716] Brian K Radak, Christophe Chipot, Donghyuk Suh, Sunhwan Jo, Wei Jiang, James C Phillips, Klaus Schulten, and Benoît Roux. Constant-pH molecular dynamics simulations for large biomolecular systems. *J. Chem. Theory Comput.*, 13:5933–5944, 2017.
- [717] Mingzhang Wang, Caitlin M. Quinn, Juan R. Perilla, Huilan Zhang, Randall Shirra Jr., Guangjin Hou, In-Ja Byeon, Christopher L. Suiter, Sherimay Ablan, Emiko Urano, Theodore J. Nitz, Christopher Aiken, Eric O. Freed, Peijun Zhang, Klaus Schulten, Angela M. Gronenborn, and Tatyana Polenova. Quenching protein dynamics interferes with HIV capsid maturation. *Nat. Commun.*, 8:1779, 2017.
- [718] Craig MacGregor-Chatwin, Melih Sener, Samuel F.H. Barnett, Andrew Hitchcock, Meghan C. Barnhart-Dailey, Karim Maghlaoui, James Barber, Jerilyn A. Timlin, Klaus Schulten, and C. Neil Hunter. Lateral segregation of Photosystem I in cyanobacterial thylakoid. *Plant Cell*, 29:1119–1136, 2017.

- [719] M. Scheurer, P. Rodenkirch, M. Siggel, R. C. Bernardi, K. Schulten, E. Tajkhorshid, and T. Rudack. Pycontact: Rapid, customizable and visual analysis of non-covalent interactions in md simulations. *Biophys. J.*, 2018. In Press.