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Education

- Ph.D. in Biophysics (2001, Suma Cum Laude), University of Heidelberg, Germany – Molecular modelling study of the biological role of retinal Schiff base in retinal proteins
- Ph.D. program in Medicinal Chemistry (1989-1995), School of Pharmacy, Tehran University, Iran (*First rank in the Final Comprehensive Board Exam for last year Ph.D. students*) – Structure activity relationship of L-type calcium channel blockers
- Doctorate of Pharmacy (Pharm. D.) (1983-1989), School of Pharmacy, Tehran University, Iran - Thesis in Pharmacology: pharmacological characterization of chicken expansor muscle
- Diploma in Mathematics and Physics (1978-1982), Kharazmi High School, Tehran, Iran.

Awards and Honors

- Winner of the *2004 Visualization Contest organized by the Science magazine and NSF* published in ***Science*** *305, 1905 (2004).*
- An animation displaying the results of my simulation studies on aquaporin water channels is deposited at the Nobel Museum web site, in conjunction to the 2003 Nobel Prize in Chemistry. http://nobelprize.org/chemistry/laureates/2003/animations.html

Professional experience

- **Assistant Director for Research**, NIH Resource for Macromolecular Modeling and Bioinformatics, Beckman Institute, University of Illinois at Urbana-Champaign; July 2001-
- **Postdoctoral research associate**, Theoretical Biophysics Group, Beckman Institute, University of Illinois at Urbana-Champaign; July 2000-July 2001
- **Research fellow**, Department of Theoretical Physics, University of Paderborn, Paderborn, Germany; Jan 2000-Jul 2000
- **Postdoctoral Fellow**, Dept. Mol. Biophysics, German Cancer Research Center, Heidelberg, Germany; 1996-1999
- **Chemistry, Organic Chemistry and Medicinal Chemistry instructor**, School of Pharmacy, Tehran University of Medical Sciences; 1989-1995
- **Counseling Pharmacist**, Central Pharmacy of Tehran University; 1987-1995

- Editorial Board of International J. Molecular Science; 1999-
- Member of the Federation of American Societies for Experimental Biology, 2001-
- Member of the American Biophysical Society, 2000-
- Member of the Iranian Medical Council, 1990-
- Member of the Iranian Society of Pharmacists, 1991-

Technical Skills

- Classical MD simulations
- Homology modeling of proteins
- Modeling of carbohydrate chains
- Modeling of proteins in membrane
- Calculation of quantum mechanical potential energy surfaces
- Implicit and explicit solvation
- Hybrid QM/MM calculations
- Study of proton transfer

- Grant proposal: Preparation of several grant proposals submitted to NIH, NSF, EC, DFG, and Human Frontier Science Program, as well as computer time proposals submitted to NCSA and PSC.

Teaching experience

- Biophysics of Membrane Proteins (Graduate course, UIUC, Biophysics, Winter 2003)
- Summer School for Theoretical and Computational Biophysics (UIUC, Beckman, June 2003, Oct 2004, Nov 2004)
- Pharmacology (Nursing and Pharmacy students, Tehran, 1994-1995)
- Chemistry and Medicinal Chemistry (Pharmacy students, Tehran University, 1993-1994)

References

- **Klaus Schulten, PhD**
  Professor of Physics
  Department of Physics and Beckman Institute
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- **Sándor Suhai, PhD**
  Head and Professor of Biophysics
  Department of Molecular Biophysics, German Cancer Research Center
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  Email: S.Suhai@dkfz-Heidelberg.de

- **Z. Luthey-Schulten, PhD**
  Department of chemistry
  Chemical and Life Sciences Laboratory, MC-712
  600 South Mathews Avenue,
  Urbana, IL 61801-3364
  Tel: (217) 333-3518; Fax: (217) 244-3186
  Email: zan@uiuc.edu

Publications

2004

1. N. Chakrabarti, *E. Tajkhorshid*, B. Roux, and R. Pomes (2004) Molecular basis of proton blockage in aquaporins. ***Structure***, 12, 65-74.
2. F. Zhu, *E. Tajkhorshid*, and K. Schulten (2004) Theory and simulation of water permeation in aquaporin-1. ***Biophysical Journal*** 86, 50-57.
3. B. Ilan, *E. Tajkhorshid*, K. Schulten, and G. A. Voth (2004) The mechanism of proton exclusion in aquaporin channels. ***PROTEINS: Structure, Function, and Bioinformatics*** 55:223-228.
4. F. Autenrieth, *E. Tajkhorshid*, J. Baudry, and Z. Luthey-Schulten (2004) Classical force field parameters for the heme prosthetic group of cytochrome c. ***J. Comp. Chem.*** 25:1613-1622.
5. J. Baudry, *E. Tajkhorshid*, and K. Schulten (2004) Complementarities and convergence of results in bacteriorhodopsin trimer simulations. ***Biophysical Journal*** 87:1394-1395.
6. S. Hayashi, *E. Tajkhorshid*, H. Kandori, and K. Schulten (2004) 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.
7. F. Autenrieth, *E. Tajkhorshid*, K. Schulten, and Z. Luthey-Schulten (2004) Role of water in transient cytochrome c2 docking. ***J. Phys. Chem. B*** in press.
8. S. André, H. Kaltner, M. Lensch, R. Russwurm, H.-C. Siebert, E. Tajkhorshid, A. J. R. Heck, M. von Knebel-Doeberitz, H.-J. Gabius, J. Kopitz (2004) Determination of structural and functional overlap/divergence of five proto-type galectins by analysis of the growth-regulatory interaction with ganglioside GM1 in silico and in vitro human neuroblastoma cells. ***Int. J. Cancer*** in press.
9. *E. Tajkhorshid*, F. Zhu, and K. Schulten (2004) Kinetic theory and simulation of single-channel water transport. In Horia Metiu, Editor, ***Handbook of Materials Modeling*** in press.
10. F. Zhu, *E. Tajkhorshid*, and K. Schulten (2004) Collective diffusion model for water permeation through microscopic channels. ***Phys. Rev. Lett.*** in press.
11. *E. Tajkhorshid*, J. Cohen, A. Aksimentiev, M. Sotomayor, and K. Schulten (2004) Towards understanding membrane channels. In ***Bacterial ion channels and their eukaryotic homologues*** Boris Martinac and Andrzej Kubalski, Editors. American Society of Microbiology. in press.

2003

12. R. Amaro, *E. Tajkhorshid*, and Z. Luthey-Schulten (2003) Developing an Energy Landscape for the Novel Function of a $(\beta/\alpha)_8$ Barrel: Ammonia Conduction through HisF. ***Proc. Natl. Acad. Sci. USA*** 100, 7599-7604.
13. *E. Tajkhorshid*, A. Aksimentiev, I. Balabin, M. Gao, B. Isralewitz, J. C. Phillips, F. Zhu, and K. Schulten (2003) Large scale simulation of protein mechanics and function. In David Eisenberg and Peter Kim, editors, ***Advances in Protein Chemistry*** 66, 195-247. Elsevier Academic Press, New York, 2003.
14. P. Grayson, *E. Tajkhorshid*, and K. Schulten (2003) Mechanisms of selectivity in channels and enzymes studied with interactive molecular dynamics. ***Biophysical Journal*** 85, 36-48.
15. S. Hayashi, *E. Tajkhorshid*, and K. Schulten (2003) Molecular dynamics simulation of bacteriorhodopsin's photoisomerization using ab initio forces for the excited chromophore. ***Biophysical Journal*** 85, 1440-1449.
16. S. Park, F. Khalili-Araghi, *E. Tajkhorshid*, and K. Schulten (2003) Free energy calculation from nonequilibrium molecular dynamics simulations using Jarzynski's equality. ***Journal of Chemical Physics*** 119:3559-3566.

17. M. Ø. Jensen, *E. Tajkhorshid*, and K. Schulten (2003) Electrostatic tuning of permeation and selectivity in aquaporin water channels. ***Biophysical Journal*** 85, 2884-2899.

18. H.-C. Siebert, S. Andre, S.-Y. Lu, M. Frank, Herbert Kaltner, J. A. van Kuik, E. Y. Korchagina, N. Bovin, *E. Tajkhorshid*, R. Kaptein, J. F. G. Vliegenhart, C.-W. von der Lieth, J. Jimenez-Barbero, J. Kopitz, and H.-J. Gabius (2003) Unique Conformer Selection of the Human Growth-regulatory Lectin Galectin-1 for Ganglioside GM1 Versus Bacterial Toxins. ***Biochemistry*** 42, 14762-14773.

2002

19. *E. Tajkhorshid*, P. Nollert, M. Ø. Jensen, L. J. W. Miercke, J. O'Connell, R. M. Stroud, and K. Schulten (2002) Control of the selectivity of the aquaporin water channel family by global orientational tuning. ***Science*** 296**,** 525-530.

20. M. Jensen, S. Park, *E. Tajkhorshid*, and K. Schulten (2002) Energetics of glycerol conduction through aquaglyceroporin GlpF. ***Proc. Natl. Acad. Sci. USA*** 99, 6731-6736.

21. H. Zhou, *E. Tajkhorshid*, Th. Frauenheim, S. Suhai, and M. Elstner (2002) Performance of the AM1, PM3, and SCC-DFTB methods in the study of conjugated Schiff base molecules. ***Chemical Physics*** 277**,** 91-103.

22. F. Zhu, *E. Tajkhorshid*, and K. Schulten (2002) Pressure-induced water transport in membrane channels studied by molecular dynamics. ***Biophysical Journal*** 83, 154-160.

23. S. Hayashi, *E. Tajkhorshid*, and K. Schulten (2002) Structural changes during the formation of early intermediates in the bacteriorhodopsin photocycle. ***Biophysical Journal*** 83, 1281-1297.

24. S. Hayashi, *E. Tajkhorshid*, and K. Schulten (2002) Structure and spectral tuning mechanism of photo-sensory protein sRII (pR). ***Biophysics (Seibutsu-Butsuri)*** 42, 127-130.

25. J. Saam, *E. Tajkhorshid*, S. Hayashi, and K. Schulten. (2002) Molecular dynamics investigation of primary photoinduced events in the activation of rhodopsin. ***Biophysical Journal*** 83, 3097-3112.

2001

26. M. Ø. Jensen, *E. Tajkhorshid*, and K. Schulten (2001) The Mechanism of Glycerol Conduction in Aquaglyceroporins. ***Structure*** 9, 1083-1093. (featuring the cover page figure)

27. J. Baudry, *E. Tajkhorshid*, F. Molnar, J. C. Phillips, and K. Schulten (2001) Molecular dynamics study of bacteriorhodopsin and the purple membrane. Invited feature article, ***Journal of Physical Chemistry B*** 105, 905-918. (featuring the cover page figure)

28. F. Zhu, *E. Tajkhorshid*, and K. Schulten (2001) Molecular Dynamics Study of Aquaporin-1 Water Channel in a Lipid Bilayer. ***FEBS Letters*** 504, 212-218.

29. S. Hayashi, *E. Tajkhorshid*, E. Pebay-peyroula, A. Royant, E. M. Landau, J. Navarro, and K. Schulten (2001) Structural determinants of spectral tuning in retinal proteins - bacteriorhodopsin *vs.* sensory rhodopsin II. ***Journal of Physical Chemistry B*** 105, 10124-10131. (featuring the cover page figure)

30. K. J. Jalkanen, R. M. Nieminen, K. Frimand, J. Bohr, H. Bohr, R. Wade, E. Tajkhorshid, and S. Suhai **(**2001**)** A comparison of aqueous solvent models used in the calculation of the Raman and ROA spectra of L-alanine. ***Chemical Physics*** 265, 125-151.

31. H. C. Siebert, *E. Tajkhorshid*, and J. Dabrowski (2001) Barriers to rotation around the C_{sp2}-C_{sp2} bond of the ketoaldehyde enol ether MeC(O)=CH-OEt as determined by ^{13}C NMR and *ab initio* calculation. ***Journal of Physical Chemistry A*** 105, 8488-8494.

2000

32. *E. Tajkhorshid*, J. Baudry, K. Schulten, and S. Suhai **(**2000**)** Molecular dynamics study of the nature and origin of the retinal's twisted structure in bacteriorhodopsin. ***Biophysical Journal*** 76**,** 683-693.

33. *E. Tajkhorshid* and S. Suhai **(**2000**)** The dielectric effects of the environment on the pK_a of the retinal Schiff Base and on the stabilization of the ion pair in bacteriorhodopsin. ***THEOCHEM J. Mol. Structure***, 501-502, 297-313.

1999

34. *E. Tajkhorshid*, B. Paizs, and Suhai S. **(**1999**)** Role of isomerization barriers in the pK_a control of the retinal Schiff base: a density functional study. ***J. Phys. Chem. B***, 103, 4518-4527.

35. W. Han, *E. Tajkhorshid*, and S. Suhai **(**1999**)** *Ab initio*/molecular mechanics study of active site of free papain and NMA-papain complex. ***J. Biomolecular Structure and Dynamics***, 16, 1019-1032.

36. *E. Tajkhorshid* and S. Suhai **(**1999**)** Dielectric effects due to the protein environment on the structure and proton affinity of the retinal Schiff base. ***Chem. Phys. Lett.***, 299, 457-464.

37. *E. Tajkhorshid* and S. Suhai **(**1999**)** Influence of the methyl groups on the structure, charge distribution, and proton affinity of the retinal Schiff base. ***J. Phys. Chem. B***, 103, 5581-5590.

38. *E. Tajkhorshid* and S. Suhai **(**1999**)** The effect of the protein environment on the structure and charge distribution of the retinal Schiff base in Bacteriorhodopsin. ***Theoret. Chem. Accounts***, 101, 180-185.

39. B. Paizs, *E. Tajkhorshid*, and S. Suhai **(**1999**)** Electronic effects on the ground state rotational barrier of the chromophore in bacteriorhodopsin: a molecular orbital study. ***J. Phys. Chem. B***, 103, 5388-5395.

1998 and earlier

40. *E. Tajkhorshid*, K. J. Jalkanen, and S. Suhai **(1998)** A density functional study of the structures and vibrational spectra of the zwitterion L-alanine in the presence of explicit water molecules. ***J. Phys. Chem. B***, 102, 5899-5913.

41. C.-W. von der Lieth, H.-C. Siebert, T. Kozar, M. Burchert, M. Frank, M. Gilleron, H. Kaltner, G. Kayser, *E. Tajkhorshid*, N. V. Bovin, J. F. G. Vliegenthart, and H.-J. Gabius **(1998)** Lectin ligands: New insights into their conformations and their dynamic behavior and the discovery of conformer selection by lectins. ***Acta Anatomica***, 161, 91-109.

42. *E. Tajkhorshid*, B. Paizs, and S. Suhai **(1997)** Conformational effects on the proton affinity of the Schiff Base in bacteriorhodopsin: a density functional study. ***J. Phys. Chem. B***, 101, 8021-8028.

43. H.-C. Siebert, R. Adar, R. Arango, M. Burchert, H. Kaltner, G. Kayser, *E. Tajkhorshid*, C.-W. von der Lieth, R. Kaptein, N. Sharon, J. F. G. Vliegenthart, and H.-J. Gabius **(1997)** Involvement of laser photo CIDNP-reactive amino acid side chains in ligand binding by galctoside-specific lectins in solution. Similarities in the role of tryptophan/tyrosine residues for ligand binding between a plant agglutinin and mammalian/avian galectins and the detection of an influence of single-site mutagenesis on surface presentation of spatially separated residues. ***Eur. J. Biochem.***, 249, 27-38.

44. *E. Tajkhorshid*, H.-C. Siebert, M. Burchert, H. Kaltner, G. Kayser, C.-W. von der Lieth, R. Kaptein, J. F. G. Vliegenthart, and H.-J. Gabius **(1997)** A combined molecular modeling and CIDNP study of similarities in the pattern of ligand binding in mammalian and avian galectins. ***J. Mol. Model.***, 3, 325-331.

45. I. Yavari, *E. Tajkhorshid*, D. Nourishargh, and S. Balalaie **(1997)** Semiempirical SCF-MO study of bowl-to-bowl inversion in corannulene and smaller circulenes. ***THEOCHEM J. Mol. Structure***, 393, 163-166.

46. H.-C. Siebert, *E. Tajkhorshid*, C.-W. von der Lieth, R. Kleineidam, S. Kruse, R. Schauer, R. Kaptein, H.-J. Gabius, and J. F. G. Vliegenthart **(1996)** Knowledge-based homology modeling and experimental determination of amino acid side chain accessibility by the laser photo CIDNP (chemically induced dynamic nuclear polarization) approach in solution: lessons from the small sialidase of Clostridium perfringens. ***J. Mol. Model.***, 2, 446-455.

47. N. Radjaee-Behbahani, A. R. Dehpour, *E. Tajkhorshid*, and K. Kheirollahi **(1996)** Clonidine-induced rhythmic activity in rabbit annococcygeus muscle. ***Gen. Pharmacol.***, 27, 525-528.

48. A. R. Dehpour, *E. Tajkhorshid*, A. Alimian, and N. Radjaee-Behbahani **(1995)** Different calcium dependencies of contractile activity of prostatic and epididymal portions of rat vas deferens. ***Gen. Pharmacol.***, **26**, 633-639.

49. A. R. Dehpour, *E. Tajkhorshid*, and N. Radjaee-Behbahani **(1994)** The role of calcium and alpha-adrenoceptors in contractile response of chick expansor secundariorum muscle to field stimulation. ***Gen. Pharmacol.***, **25**, 317-323.

50. A. R. Dehpour, *E. Tajkhorshid*, N. Radjaee-Behbahani, and K. Kheirollahi **(1993)** Methoxamine-induced rhythmic activity in rabbit annococcygeus muscle. ***Gen. Pharmacol.***, **24**, 841-845.

51. *E. Tajkhorshid*, B. Habibi-Nezhad, and P. Rashidi-Ranjbar **(1992)** Successes of computer-aided molecular design. ***Iran. J. Chem. Chem. Engineering***, **11**, 86-100.

Lectures and Seminars

- Mechanism of Storage of Light Energy in Rhodopsins (**Sep 2004**) Invited lecture at the *International Symposium on Retinal Proteins: Experimental and Theory*, Heidelberg, Germany.
- Novel Mechanisms of Substrate Selectivity in Membrane Channels (**Sep 2004**) Invited lecture at the *2004 Annual Meeting of the German Biophysical Society*, Freiburg, Germany.
- Selective Transport of Substrates across Biological Membranes: Lessons from Computational Studies of Membrane Channels (**Jun 2004**) Invited lecture at the Department of Medicine, University of Chicago, Chicago, Illinois, USA.
- Structural Basis of Substrate Permeation and Selectivity in Membrane Channels: Lessons from Non-Equilibrium Simulations (**Feb 2004**) Invited lecture at the *Permeation/Transport Subgroup* of the *48th Annual Meeting of the Biophysical Society*, Baltimore, Maryland, USA.
- Electrostatics Regulation of Substrate Permeation and Selectivity of Aquaporins. (**Feb 2004**) *48th Annual Meeting of the Biophysical Society*, Baltimore, Maryland, USA.
- Largest-Scale Full-Atomic Simulations of Biomolecular Processes (**Nov 2003**) Invited lecture at "Multi-scale simulation of biological systems, *International Conference on Systems Biology 2003"*, St. Louis, MI, USA.
- Molecular mechanisms of photoactivation and spectral tuning in retinal proteins (**Oct 2003**) Invited lecture at *"Software Solutions to Large Scale Problems in Computational Chemistry" Computational Chemistry GRID Conference*, University of Kentucky, Lexington, Kentucky, USA.
- Large Scale Molecular Dynamics Simulations of Membrane Proteins. (**Jul 2003**) Invited lecture at *Computing for Biology, IBM-BNL Blue-Gene Science Workshop 2003*. Long Island, New York, USA.
- Computational Studies of Aquaporin Function and Mechanism. (**Jun 2003**) Invited lecture at Gordon Research Conference on Mechanisms of Membrane Transport, Holderness, New Hampshire, USA.
- Novel Selectivity Mechanisms of Membrane Channels: Insights from Computational Investigations of Aquaporins. (**May 2003**) Invited lecture at *Department of Molecular and Integrative Physiology*, University of Illinois at Urbana-Champaign, Urbana, Illinois, USA.
- Molecular dynamics simulation of aquaporin mutants in congenital cataracts. (**Mar 2003**) *47th Annual Meeting of Biophysical Society*, San Antonio, Texas, USA.
- Computational Modeling of Substrate Transport Through Membrane Channels (**Feb 2003**) Invited lecture at *43rd Sanibel Symposium*, St Agustine, Florida, USA.
- Architectural Design of a Highly Selective Membrane Channel. (**Oct 2002**) Molecular and Electronic Nanostructures Seminar Series (Nanohour), Beckman Institute for Advanced Science and Technology, University of Illinois at Urbana-Champaign, Urbana, Illinois, USA.
- Large scale molecular dynamics simulation of biomolecular systems. (**Oct 2002**) Invited lecture at *"Software Solutions to Large Scale Problems in Computational Chemistry" Computational Chemistry GRID Conference*, University of Kentucky, Lexington, Kentucky, USA.
- Computational chemistry for membrane channels. (**Jul 2002)** Invited lecture at *Gordon Research Conference* on Computational Chemistry, Colby-Sawyer College, New London, New Hampshire, USA.
- Aquaporin membrane channels. (**Apr 2002**) NCSA Workshop on "Biomedical Applications of Molecular Dynamics on the TeraGrid", *NCSA, University of Illinois at Urbana-Champaign*, Urbana, Illinois, USA.
- Computational exploration of structure-function relationship in aquaporin water channels (**Feb 2002**) Invited lecture at Chemical Biology Seminars, *University of Illinois at Urbana-Champaign*, Urbana, Illinois, USA.

- Structural determinants of spectral tuning in retinal proteins (**Aug 2001**) *German Cancer Research Center*, Heidelberg, Germany.
- Exploring Glycerol and Water Transport in the *E. Coli* Glycerol Facilitator (GlpF) by Molecular Dynamics Simulations. (**Jun 2001**) *German Cancer Research Center*, Heidelberg, Germany.
- Exploring the Glycerol Transport in Glpf by Molecular Dynamics Simulations (**Apr 2001**) University of California San Francisco, San Francisco, California, USA.
- Molecular basis of function in retinal proteins. (**Feb 2001**) Invited lecture at Molecular and Electronic Nanostructures Seminar Series (Nanohour), *Beckman Institute for Advanced Science and Technology, University of Illinois at Urbana-Champaign*, Urbana, Illinois, USA.
- Simulation of the structure and function of retinal proteins. (**2000**) Invited lecture at *Departemnt of Physics, Central Michigan University*, Mt. Pleasent, Michigan, USA.
- Theoretical study of the interaction of chromophore and protein environment in bacteriorhodopsin (**2000**) *Workshop on Theoretical studies of biological function of molecules, University of Paderborn*, Paderborn, Germany.
- Theoretical study of the structure and function of the retinal chromophore in bacteriorhodopsin. (**2000**) Invited lecture at *University of Freiburg*, Freiburg, Germany.
- The central role of the retinal Schiff base in the photoabsorption and proton transfer activities of bacteriorhodopsin. (**2000**) *University of Paderborn*, Paderborn, Germany.
- Interaction of retinoids with their biological receptive sites. **(1999)** *German Cancer Research Center*, Heidelberg, Germany.
- The effect of different structural characteristics of the retinal Schiff base on the isomerization barriers and the pK_a of the chromophore. **(1998)** *Beckman Institute for Advanced Science and Technology, University of Illinois at Urbana-Champaign*, Urbana, Illinois, USA.
- Theoretical study of the structure and electronic configuration of retinoids. **(1998)** *Supercomputing Workshop, German Cancer Research Center*, Heidelberg, Germany.
- Conformational analysis of zwitterionic form of L-alanine in aqueous solution. **(1996)** *German Cancer Research Center*, Heidelberg, Germany.
- Developmental changes of chick expansor secundariorum muscle sensitivity to 5-hydroxytryptamine. **(1991)** *10th Iranian Congress of Physiology and Pharmacology*, Ahwaz, IRAN.