Giray Enkavi

CONTACT

Biological Physics & Soft Matter (BIO) Group
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Tampere University of Technology
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EDUCATION

PhD in Biophysics and Computational Biology — Sep 2007 — Dec 2013

University of Illinois at Urbana-Champaign, USA

Doctoral Advisor: Prof. Emad Tajkhorshid
Dissertation: Mechanism and Energetics of Membrane Transporters and Channels

BSc (Double Major) in Molecular Biology and Genetics & Physics — Sep 2003 — Jun 2007

Boğaziçi University, Turkey

WORK EXPERIENCE

Tampere University of Technology — Aug 2014 — Present

Postdoctoral Researcher

Biological Physics & Soft Matter (BIO) Group
Postdoctoral Advisor: Prof. Ilpo Vattulainen

University of Illinois at Urbana-Champaign — Jan 2014 — Aug 2014

Postdoctoral Research Associate

Computational Structural Biology and Molecular Biophysics Group
Postdoctoral Advisor: Prof. Emad Tajkhorshid

University of Illinois at Urbana-Champaign — Jan 2008 — Dec 2013

Graduate Research Assistant

Computational Structural Biology and Molecular Biophysics Group
Graduate Advisor: Prof. Emad Tajkhorshid

University of Illinois at Urbana-Champaign — Jan 2010 — May 2010

Graduate Teaching Assistant

Computational Structural Biology Course

RESEARCH AND TEACHING EXPERIENCE

- Molecular dynamics simulations of mebrane-protein interactions (present)
- Molecular dynamics simulations of membrane transporters and channels (2007-present)
- Knowledge and molecular dynamics based modeling of alternate conformations of membrane proteins (2009-Present)
- Estimation of free energies of alternate conformations of membrane transporters (2010-Present)
- Teaching assistant at 'Hands-On' Workshop on Computational Biophysics at Jacobs University Bremen, Germany (Oct, 2011)
- Teaching assistant at biannual 'Hands-On' Workshops on Computational Biophysics, Urbana (2009-Present)
- Teaching assistant for Computational Structural Biology Course, UIUC (Spring, 2010)
- Summer research trainee at Hacettepe University Ankara, Turkey, Supervisor: Erhan Piskin, Bioengineering Graduate Program and Biomedical Technologies Center (Summer, 2006)
- Private tutoring to high school and college students (2004-2007)

COMPUTER SKILLS

Shell scripting (Unix/Linux), MATLAB, Python, NAMD, VMD, MODELLER, AutoDock, Gromacs

HONORS AND SCHOLORSHIPS

- Travel Award from the Gordon Research Conference on Mechanisms of Membrane Transport (2011)
- Gregorio Weber Fellowship in Biophysics (Fall, 2007)
- Scholarship of Achievement from the Scientific & Technological Research Council of Turkey (2004 -2007)
- Scholarship of Achievement at Uskudar American Academy and FMV Işık High School (1995-2003)

PUBLICATIONS

- G. Enkavi, J. Li, P.-C. Wen, S. Thangapandian, M. Moradi, T. Jiang, W. Han, and E. Tajkhorshid (2014) A Microscopic View of the Mechanisms of Active Transport Across the Cellular Membrane. **Annual Reviews in Computational Chemistry**, in press.
- J. Li, G. Enkavi, P.-C. Wen, S. A. Shaikh, and E. Tajkhorshid (2013) Transient Formation of Water-conducting States in Membrane Transporters. **Proceedings of the National Academy of Sciences USA**, 110: 7696-7701.
- U. K. Eriksson, G. Fischer, R. Friemann, G. Enkavi, E. Tajkhorshid*, and R. Neutze* (2013) Sub-Angstrom resolution x-ray structure details aquaporin-water interactions. **Science**, 340: 1346-1349.
- S. A. Shaikh, J. Li, G. Enkavi, P.-C. Wen, Z. Huang, and E. Tajkhorshid (2013) Visualizing Functional Motions of Membrane Transporters with Molecular Dynamics Simulations. **Biochemistry** (Current Topic) 52: 569-587.
- R. R. Geyer, R. Musa-Aziz, G. Enkavi, P. Mahinthichaichan, E. Tajkhorshid, and W. Boron (2013) Movement of NH3 through the Human Urea Transporter B (UT-B): A New Gas Channel. **American Journal of Physiology - Renal Physiology**, 304: F1447-F1457.
- G. Enkavi, J. Li, P. Mahinthichaichan, P.-C. Wen, Z. Huang, S. A. Shaikh, and E. Tajkhorshid (2013) Simulation Studies of the Mechanism of Membrane Transporters. In Editors: Luca Monticelli and Emppu Salonen,

"Biomolecular Simulations – Methods and Protocols", Humana Press. **Methods in Molecular Biology**, Vol. 924, Part 2, 361-405.

- E. J. Levin, Y. Cao, G. Enkavi, M. Quick, Y Pan, E. Tajkhorshid*, and M. Zhou* (2012) Structure and permeation mechanism of a mammalian urea transporter. **Proceedings of the National Academy of Sciences USA**, 109: 11194-11199.
- Z. Huang, S. A. Shaikh, P.-C. Wen, G. Enkavi, J. Li, and E. Tajkhorshid (2011) Membrane Transporters - Molecular Machines Coupling Cellular Energy to Vectorial Transport Across the Membrane. **In Editor: Benoit Roux, "Molecular Machines", Chapter 9: pp. 151–182**, World Scientific Publishing, Singapore.
- G. Enkavi and E. Tajkhorshid (2010) Simulation of spontaneous substrate binding revealing the binding pathway and mechanism and initial conformational response of GlpT. **Biochemistry**, 49: 1105-1114.
- P.-C. Wen, Z. Huang, G. Enkavi, Y. Wang, J. C. Gumbart, and E. Tajkhorshid (2010) Molecular mechanisms of active transport across the cellular membrane. **In, Editors: Mark Sansom and Philip Biggin, "Molecular Simulations and Biomembranes: From Biophysics to Function"** pp. 248-286. Royal Society of Chemistry, Cambridge, UK.
- S. Shaikh, P.-C. Wen, G. Enkavi, Z. Huang, and E. Tajkhorshid (2010) Capturing Functional Motions of Membrane Channels and Transporters with Molecular Dynamics Simulation. **Journal of Computational and Theoretical Nanosciences**, 7;2481-2500.
- J. Feng, E. Lucchinetti, G. Enkavi, Y. Wang, P. Gehrig, B. Roschitzki, M. C. Schaub, E. Tajkhorshid, K. Zaugg, and M. Zaugg (2010) Tyrosine phosphorylation by Src within the cavity of the adenine nucleotide translocase 1 regulates ADP/ATP exchange in mitochondria. **American Journal of Physiology - Cell Physiology**, 298: 740-748.
- Ch. Law*, G. Enkavi*, D.-N. Wang, and E. Tajkhorshid (2009) Structural basis of substrate selectivity in the glycerol-3-phosphate:phosphate antiporter GlpT. **Biophysical Journal**, 97: 1346-1353. *equal contribution

SELECTED CONFERENCE PRESENTATIONS

- Transport Cycle of Mitochondrial Carriers from Internal Symmetries. Giray Enkavi, Emad Tajkhorshid. Poster presented at the Biophysical Society 56th Annual Meeting, San Diego, 2012.
- Permeation and Selectivity of Urea Transporters. Giray Enkavi, Elena J. Levin, Ming Zhou, Emad Tajkhorshid. Talk given and poster presented at the Gordon Research Conference on Mechanisms of Membrane Transport, Biddeford, 2011.
- Energetics and Molecular Mechanisms of Permeation and Selectivity of Transport in the Urea Transporter. Giray Enkavi, Elena J. Levin, Ming Zhou, Emad Tajkhorshid. Poster presented at the Biophysical Society 55th Annual Meeting, Baltimore, 2011.
- Molecular Determinants of the Stoichiometry of Transport in GlpT. Giray Enkavi, Emad Tajkhorshid. Poster presented at the Biophysical Society 54th Annual Meeting, San Francisco, 2010.
- Spontaneous Substrate Binding and Formation of the Bound State in Glycerol-3-Phosphate Transporter (GlpT). Giray Enkavi, Emad Tajkhorshid. Poster presented at the Biophysical Society 53rd Annual Meeting, Boston, 2009.
- Spontaneous substrate binding and formation of the bound state in GlpT. Giray Enkavi and Emad Tajkhorshid. Talk given at the Cell and Molecular Biology & Molecular Biophysics Training Grants - 21st Annual Research Symposium, Urbana, 2008.