

CURRICULUM VITAE

Andrzej Kloczkowski
Battelle Center for Mathematical Medicine
Abigail Wexner Research Institute at Nationwide Children's Hospital and
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Contact Information

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Research Interests

Biophysical chemistry and bioinformatics.
Biopolymers, proteins and nucleic acids.
Protein folding and prediction of protein structure and function from the amino acid sequence.
Modeling of dynamics of large biological structures, such as ribosome, with Elastic Network Models.
Development of computational, graphical, statistical and mathematical, or algorithmic methods to interpret or mine information from biological data.
Prediction of post-translational modification sites in proteins.
Improvement of protein contact potentials.
Development of 3-D threading for automatic function annotation.
Systems biology. Applications of various graph-theoretical concepts from theory of polymer networks to metabolic and protein-protein interaction networks.

Education

June 1974	M.Sc. (Physical Chemistry), Warsaw University (Honors: Magna Cum Laude)
June 1980	Ph.D. (Statistical Thermodynamics), Institute of Physical Chemistry of the Polish Academy of Sciences. (Thesis: Statistical Mechanics of Liquid Crystals. Advisor: Prof. Jan Stecki)
Dec 2001	Habilitation (D.Sc.) (Physical Chemistry), Warsaw University

Brief Chronology of Employment

1981 - 1983	Postdoctoral Research Associate, Stanford University
1983 - 1987	Assistant Professor, Institute of Physical Chemistry of the Polish Academy of Sciences
1987 - 1995	Research Associate, Department of Chemistry, University of Cincinnati
1995 - 1997	Senior National Research Council Fellow Laboratory of Mathematical Biology, NCI, NIH
1997 - 2002	Senior Staff Fellow, Laboratory of Experimental and Computational (Mathematical) Biology, NCI, NIH
2002 - 2007	Scientist I, Baker Center for Bioinformatics and Biological Statistics, Iowa State University

2008 - 2010	Scientist II, Baker Center for Bioinformatics and Biological Statistics, Iowa State University
2006 - 2010	Adjunct Professor, Department of Biochemistry, Biophysics and Molecular Biology, Iowa State University
2010-present	Collaborator Professor, Department of Biochemistry, Biophysics and Molecular Biology, Iowa State University
2011-present	Professor, Department of Pediatrics (tenured since April 1, 2011) The Ohio State University, College of Medicine
2010-present	Principal Investigator II, Battelle Center for Mathematical Medicine The Research Institute at Nationwide Children's Hospital

Societies

American Association for the Advancement of Science
American Chemical Society
Association for Computing Machinery
Biophysical Society
Protein Society

Honors & Other Special Scientific Recognition

1969 Winner of the National Chemistry Olympiad for high school students
1981 Excellence Award of the Scientific Secretary of the Polish Academy of Sciences for the Ph.D. Thesis
1986 British Council Fellowship Award
1986 Humboldt Foundation Fellowship Award
1999 NIH Fellows Award for Research Excellence

Editorial Boards

International Journal of Molecular Sciences (Molecular Biophysics Section)
Computational and Mathematical Methods in Medicine
Journal of Glycomics & Lipidomics
Metabolomics: Open Access
Annual Review & Research in Biology

Organized Conferences

Coarse-Grained Modeling of Structure and Dynamics of Biomacromolecules, Telluride, CO, June 5-9, 2010, Co-organizer

The First Immunoinformatics and Computational Immunology Workshop (ICIW2010) at the ACM International Conference on Bioinformatics and Computational Biology (ACM-BCB), Niagara Falls, NY, August 2-4, 2010, Program Committee Member

International Conference on Bioinformatics - BIOINFORMATICS 2011, Rome, Italy, January 26-29, 2011, Program Committee Member

The Second Immunoinformatics and Computational Immunology Workshop (ICIW2011) at the ACM International Conference on Bioinformatics and Computational Biology (ACM-BCB), Chicago, IL, August 1-3, 2011, Program Committee Member

2011 International Conference on Computational Biology and Bioinformatics (CBB2011), Shanghai, China, October 28-30, 2011, Technical Program Committee Member

Zing Conference on Protein and RNA Structure Prediction, Xcaret, Mexico, December 3-7, 2011, Organizer and Chair

International Conference on Bioinformatics Models, Methods and Algorithms - BIOINFORMATICS –BIOSTEC 2012, Vilamoura, Algarve, Portugal, February 1-4, 2012, Program Committee Member

2012 Spring World Congress on Engineering and Technology (SCET), Xi'an, China, May 26-29, 2012, Technical Program Committee Member

Coarse-Grained Modeling of Structure and Dynamics of Biomacromolecules, Telluride, CO, July 23-27, 2012, Organizer

The Third Immunoinformatics and Computational Immunology Workshop (ICIW2012) at the ACM International Conference on Bioinformatics and Computational Biology (ACM-BCB), Orlando, FL, October 7-10, 2012, Program Committee Member

Zing Conference on Computational Medicine, Xcaret, Mexico, December 1-5, 2012, Organizer and Chair

International Society for Computational Biology ISCB-Asia/SCCG 2012, Dameisha Beach, Shenzhen, China December 17-19, 2012, Editor/Program Committee Member

International Conference on Bioinformatics Models, Methods and Algorithms - BIOINFORMATICS – BIOSTEC 2013, Barcelona, Spain, February 11-14, 2013, Program Committee Member

International Congress on Neurotechnology, Electronics and Informatics - NEUROTECHNIX 2013, Vilamoura, Algarve, Portugal, September 18-20, 2013, Program Committee Member

20th Annual International Conference on Intelligent Systems for Molecular Biology ISMB 2013 Berlin July 21-23, 2013, Program Committee Member

International Conference on Omics Studies 2013, Orlando, FL September 4-6, 2013, Organizing Committee Member

The Fourth Immunoinformatics and Computational Immunology Workshop (ICIW 2013) at ACM International Conference on Bioinformatics and Computational Biology (ACM-BCB), Washington DC, Sept 23-25, 2013, Program Committee Member

Bio Molecular Eng 2013 International Conference and Exhibition on Biochemical & Molecular Engineering, October 7-9, 2013, San Antonio, Texas, Organizing Committee Member

GTC Next Generation Sequencing Conference, Berlin, Germany, October 7-11, 2013, Advisory Board Member

2nd Zing Conference on Protein and RNA Structure Prediction, Xcaret, Mexico, December 1-5, 2013, Organizer and Chair

International Conference on Physiological Computing Systems - PhyCS 2014, Lisbon, Portugal, Jan 7-9, 2014, Program Committee Member

5th International Conference on Bioinformatics Models, Methods and Algorithms – BIOINFORMATICS-BIOSTEC 2014, Eseo, Angers, Loire Valley, France, March 3-6, 2014, Program Committee Member

Great Lakes Bioinformatics Conference GLBIO 2014, Cincinnati Children's Hospital, University of Cincinnati, May 16-18, 2014, Program Committee Member

4th IEEE International Conference on Computational Advances in Bio and Medical Sciences (ICCABS), Miami Beach Resort and Spa, Miami Beach, FL, June 2-4, 2014, Program Committee Member

Coarse-Grained Modeling of Structure and Dynamics of Biomacromolecules, Telluride, CO, August 4-8, 2014, Organizer

Zing Conference on Protein Folding, Punta Cana, Dominican Republic, July 16-19, 2014, Organizer and Chair

2nd International Congress on Neurotechnology, Electronics and Informatics NEUROTECHNIX 2014, Rome, Italy, Oct 25-26, 2014.

2nd Zing Conference on Mathematical and Computational Medicine, Cancun, Mexico, Dec 1-4, 2014, Organizer and Chair

International Conference on Physiological Computing Systems PhyCS 2015, Angers, France, Feb 11-13, Program Committee Member

From Computational Biophysics to Systems Biology (CBSB15) Oklahoma City, May 17-19, 2015, Advisory Committee Member

2015 Great Lakes Bioinformatics Conference (GLBIO) Purdue University, May 18-20, 2015, Program Committee Member

GTC 2nd Next Generation Sequencing and Bioinformatics Conference, October 5-7, 2015, Berlin, Germany, Scientific Advisory Board Committee Member

5th IEEE International Conference on Computational Advances in Bio and Medical Sciences (ICCABS), October 15-17, 2015, Miami, FL, Program Committee Member

3rd International Conference on Protein and RNA Structure Prediction, Punta Cana, Dominican Republic, December 14-18, 2015, Organizer and Chair

3rd International Conference on Mathematical and Computational Medicine, Columbus, OH, May 16-18, 2016, Co-Organizer and Co-Chair

2016 Great Lakes Bioinformatics Conference and Canadian Computational Biology Conference (GLBIO/CCBC), University of Toronto, Canada, May 16-19, 2016, Program Committee Member

Coarse-Grained Modeling of Structure and Dynamics of Biomacromolecules, Workshop, Telluride, CO; July 25-29, 2016, Organizer

3rd International Conference on Physiological Computing Systems (PhyCS) 2016, Lisbon, Portugal, July 29-31, 2016 - Program Committee Member

6th IEEE International Conference on Computational Advances in Bio and Medical Sciences, ICCABS 2016, October 13-15, 2016, Georgia Institute of Technology, Atlanta, GA, Program Committee Member

1st International Conference on Genomics and Proteomics, Guanacaste, Costa Rica, October 18-23, 2016, Organizer and Chair

Biomolecules and Nanostructures 6, Podlesice, Poland, May 10-14, 2017 – International Advisory Board Member

4th International Conference on Physiological Computing Systems (PhyCS) 2017, Madrid, Spain, July 28-29, 2017 - Program Committee Member

International Society for Computational Biology / European Conference on Computational Biology ISMB/ECCB 2017 Conference, Prague, Czech Republic, July 21-25, 2017 - Program Committee Member

2nd International Conference on Genomics and Proteomics, Playa Blanca, Panama, August 14-18, 2017, Organizer and Chair

4th International Conference on Protein and RNA Structure Prediction, Montego Bay, Jamaica, December 4-8, 2017, Organizer and Chair

International Conference & Exhibition on Genome Science (ICEGS-2018) Jan 29-31, 2018, Las Vegas, NE, Program Committee Member

Coarse-Grained Modeling of Structure and Dynamics of Biomacromolecules, Workshop, Telluride, CO; July 23-27, 2018, Organizer

4th International Conference on Mathematical and Computational Medicine, Puerto Morelos, Mexico, December 3-7, 2018., Organizer and Chair

Biomolecules and Nanostructures 7, Pomieowo, Poland, May 15-19, 2019 - International Advisory Board Member

International Conference on Mathematical Multiscale Modeling in Biology, Guanacaste, Costa Rica, October 21-25, 2019, Organizer and Chair

5th International Conference on Protein and RNA Structure Prediction, Punta Cana, Dominican Republic, December 2-6, 2019, Organizer and Chair

Coarse-Grained Modeling of Structure and Dynamics of Biomacromolecules, Workshop, Telluride, CO; August 3-7, 2020, Organizer

Invited Lectures (*since 2008*)

52nd Biophysical Society Meeting, Long Beach, CA, Feb. 5, 2008 (also co-chaired Platform Session AG: Protein Conformation)

Illinois Institute of Technology Feb. 25, 2008

University of California Riverside March 30, 2008

Protein Structural Initiative Bottlenecks Workshop, NIH, Bethesda, April 14, 2008

Texas Tech University Health Science Center April 17, 2008

North Dakota State University Jan 22, 2009

University of California Merced March 30, 2009

Michigan Technological University April 23-24, 2009

House Ear Institute University of Southern California June 2, 2009

Methods Development for Protein Structure Prediction Workshop Telluride, CO; June 15-19, 2009

J. Craig Venter Institute, Rockville, MD, January 11, 2010

The University of Toledo, Toledo, OH, March 18, 2010

2010 NIGMS Workshop: Enabling Technologies in Structure and Function, NIH, Bethesda, April 18-21, 2010

The Ohio State University, Columbus, OH, May 13, 2010.

Coarse-Grained Modeling of Structure and Dynamics of Biomacromolecules, Telluride, CO; July 4-9, 2010

IJCCI – 2nd International Joint Conference on Computational Intelligence, Valencia, Spain, October 24-26, 2010 (two invited talks presented by a graduate student Saras Saraswathi)

The Ohio State University Biophysics Program, Columbus, OH, February 28, 2011

Indiana University-Purdue University Indianapolis, IN, Oct 10, 2011

Purdue University, West Lafayette, IN, Oct 12, 2011

Multi-Pole Approach to Structural Biology Conference, Warsaw, Poland, November 16-19, 2011

Zing Conference on Protein and RNA Structure Prediction, Xcaret, Mexico, December 3-7, 2011
56th Biophysical Society Meeting, San Diego, CA, February 26, 2012
University of Cincinnati, Cincinnati, OH, May 1, 2012
Coarse-Grained Modeling of Structure and Dynamics of Biomacromolecules, Telluride, CO; July 23-27, 2012
Zing Conference on Mathematical and Computational Medicine, Xcaret, Mexico, December 1-5, 2012
Critical Assessment of Protein Structure Prediction CASP 10, Gaeta, Italy, December 9-12, 2012
20th International Molecular Medicine Tri-Conference TRI-CON 2013, San Francisco, CA, February 11-15, 2013.
GPCR-Based Drug Design: Computational and Structural Approaches, April 16-18, 2013, San Diego (presented by Marcin Pawlowski)
BIT's 4th Annual World DNA and Genome Day, April 26-27, 2013 Nanjing China. (joint work presented by Richard Ransom).
Improved potentials and scoring functions for protein structure prediction, University of Warsaw, Poland, May 13, 2013
International Conference on Biomolecules and Nanostructures 4, Pultusk, Poland, May 15-19, 2013
Rise of the Machines: Integration of experiment, simulation and theory for a mechanistic understanding of biomolecular machines, Workshop, Telluride, CO, August 5-9, 2013
International Conference on Omics Studies 2013, Orlando, FL September 4-6, 2013
2nd Zing Conference on Protein and RNA Structure Prediction, Xcaret, Mexico, December 1-5, 2013
Genome-Wide Protein Structure and Function Prediction 21st International Molecular Medicine Tri-Conference TRI-CON 2014, San Francisco, CA, February 9-14, 2014.
From Computational Physics to Systems Biology (CBSB14), Gdansk, Poland, May 25-27, 2014
Macromolecular Dynamics: Structure, Function and Diseases, Kavli Institute for Theoretical Physics China (KITPC), Institute of Theoretical Physics (ITP), Chinese Academy of Sciences (CAS), Beijing, China June 15-July 11, 2014
The 8th IUPAP International Conference on Biological Physics (IUPAP 2014) Workshop on Frontiers of Biological Physics, Beijing, China, June 18-19, 2014.
Zing Conference on Protein Folding, Punta Cana, Dominican Republic, July 16-19, 2014
Coarse-Grained Modeling of Structure and Dynamics of Biomacromolecules, Telluride, CO; August 4-8, 2014
Biophysical Society Thematic Meeting: Modeling of Biomolecular Systems Interactions, Dynamics, and Allostery: Bridging Experiments and Computations, September 10-14, 2014, Istanbul, Turkey.
Arizona State University, Center for Biological Physics, October 8, 2014
2nd Zing Conference on Mathematical and Computational Medicine, Cancun, Mexico, Dec 1-4, 2014
Institute of Physical Chemistry of the Polish Academy of Sciences, April 9, 2015.
RECOMB 2015 Conference, Warsaw, Poland April 12-15, 2015 (presented by a postdoc Sumudu Lelalanda who received the travel award).
The Ohio State University, Mathematical Biosciences Institute Colloquium, April 20, 2015.
Biomolecules and Nanostructures 5, Jarosowice, Poland, May 13-17, 2015.
GTC 2nd Next Generation Sequencing and Bioinformatics Conference, Berlin, Germany, October 5-7, 2015.
3rd International Conference on Protein and RNA Structure Prediction, Punta Cana, Dominican Republic, December 14-18, 2015.
23rd International Molecular Medicine Tri-Conference TRI-CON 2016, San Francisco, CA, March 6-11, 2016.
BIT16 Conference Bioinformatics in Torun 2016, Torun, Poland, June 16-18, 2016.
Coarse-Grained Modeling of Structure and Dynamics of Biomacromolecules, Workshop, Telluride, CO; July 25-29, 2016.
International Conference on Genomics and Proteomics, Guanacaste, Costa Rica, October 18-23, 2016.
BIT's 7th World Gene Convention 2016, Shanghai, China, November 3-5, 2016.
BIT's 8th World DNA and Genome Day-2017, April 25-27, 2017, Xi'an, China
From Computational Biophysics to Systems Biology CBSB 2017, Cincinnati, OH, May 18-20, 2017
Protein Society 31st Annual Symposium, July 24-27, 2017, Montreal, Canada, Student Talk awarded to my student Girik Malik.
2nd International Conference on Genomics and Proteomics, Playa Blanca, Panama, August 14-18, 2017
Mathematical Biosciences Institute, The Ohio State University, September 29, 2017 (Invited lecture presented by a member of my lab Eshel Faraggi)
6th Congress of the Branch of Physicochemistry, Structure and Design of Proteins, Durango, Mexico, November 6-10, 2017
4th International Conference on Protein and RNA Structure Prediction, Montego Bay, Jamaica, December 4-8, 2017

International Work-Conference on Bioinformatics and Biomedical Engineering, IWBBIO 2018, Granada, Spain, April 25-27, 2018.

International Conference on Artificial Intelligence and Soft Computing, ICAISC 2018, Zakopane, Poland, June 3-7, 2018.

Coarse-Grained Modeling of Structure and Dynamics of Biomacromolecules, Workshop, Telluride, CO; July 23-27, 2018.

University of Oklahoma, Department of Chemistry and Biochemistry, August 24, 2018.

4th Polish Korean Conference on Protein Folding: Theoretical and Experimental Approaches, Ilawa, Poland, September 9-13, 2018.

BIT's 8th Annual World Congress of Molecular and Cell Biology, October 14-16, Fukuoka, Japan

Nagoya University, Graduate School of Informatics, Future Value Creation Research Center, November 6, 2018.

Nationwide Children's Hospital Research Retreat, Columbus, OH, November 13, 2018 (short talk presented by Maksim Kouza).

BIT's 9th World Gene Convention-2018, WGC 2018, November 13-15, 2018, Singapore.

4th International Conference on Mathematical and Computational Medicine, Puerto Morelos, Mexico, December 3-7, 2018.

Biophysical Society 63rd Annual Meeting, Baltimore, MD, March 2-6, 2019, Platform: Protein Assemblies/Enzyme Function, Cofactors & Post-translational Modifications II, March 6, 2019.

26th International Molecular Medicine Tri-Conference TRI-CON 2019, San Francisco, CA, March 10-15, 2019, Data Science, Precision Medicine and Machine Learning Symposium, March 15, 2019.

BIT's 10th Anniversary World DNA Day-2019, April 25-27, 2019, Nanjing, China.

7th International Work-Conference on Bioinformatics and Biomedical Engineering IWBBIO 2019, Grenada, Spain, May 8-10, 2019, Plenary Talk.

The 4th International Conference on Computational Science and Engineering (ICCSE), The Institute for Computational Science and Technology, July 24-27, 2019, Ho Chi Minh City, Vietnam.

BIRS Workshop: Mathematics and Computer Science in Modeling and Understanding of Structure and Dynamics of Biomolecules, Banff International Research Station, Banff, Canada, August 9-11, 2019.

American Chemical Society Fall Meeting, August 25-29, 2019, San Diego, CA, Division of Polymer Chemistry, Paul Flory's "Statistical Mechanics of Chain Molecules: The 50th Anniversary of Polymer Chemistry" Symposium.

5th Polish-Korean Conference on Protein Folding, Korea Institute for Advanced Study, Seoul, Korea, September 16-18, 2019.

International Conference on Mathematical Multiscale Modeling in Biology, Guanacaste, Costa Rica, October 21-25, 2019.

5th International Conference on Protein and RNA Structure Prediction, Punta Cana, Dominican Republic, December 2-6, 2019.

19th Annual PepTalk Protein Aggregation and Emerging Analytical Tools, San Diego, CA, January 23, 2020.

Biophysical Society 64th Annual Meeting, San Diego, CA, February 15-19, 2020, Platform: Protein Assemblies Feb. 19, 2020 (talk presented by postdoc Maksim Kouza)

5th International Conference on Mathematical and Computational Medicine, Telluride, CO, June 8-12, 2020.

International Conference on Artificial Intelligence and Soft Computing, ICAISC 2020, Zakopane, Poland, June 21-25, 2020.

Coarse-Grained Modeling of Structure and Dynamics of Biomacromolecules, Workshop, Telluride, CO; August 3-7, 2020.

6th Polish Korean Conference on Protein Folding: Theoretical and Experimental Approaches, Jastrzebia Gora, Poland, September 20-24, 2020.

Invited Grant Review Panels (*since 2008*)

NIH Study Section ZRG1 BST-30(M) Washington DC Oct 29-30, 2009 - ad hoc reviewer

NSF Division of Biological Infrastructure – member of Advances in Biological Informatics virtual review panel Oct 4, 2012 – Jan 3, 2013.

NIH Study Section ZGM1 TRN-X (KR) K99 Pathway to Independence Program Panel, April 3, 2013, mail reviewer

NRC Committee on Proposal Evaluation for Allocation of Supercomputing Time for the Study of Molecular Dynamics, Fifth Round, Washington, DC, August 15, 2014 review committee member

NRC Committee on Proposal Evaluation for Allocation of Supercomputing Time for the Study of Molecular Dynamics, Sixth Round, Washington, DC, August 4, 2015 review committee member

NRC Committee on Proposal Evaluation for Allocation of Supercomputing Time for the Study of Molecular Dynamics, Eight Round, Washington, DC, August 11, 2017 review committee member

NSF Division of Biological Infrastructure, Infrastructure Capacity for Biology (ICB) program December 10, 2018, mail reviewer

NRC Committee on Proposal Evaluation for Allocation of Supercomputing Time for the Study of Molecular Dynamics, Tenth Round, Washington, DC, September 13, 2019 review committee member

NSF Graduate Research Fellowship Program 2020 Genetics, Genomics & Proteomics virtual panel January 22, 2020, review committee member

Foundation for Polish Science – multiple grants (1-3 per year) reviewed in 2010-2019

National Science Centre in Poland - multiple grants (1-2 per year) reviewed in 2010-2019

Research Grants

Misfoldome-Centered MultiOMICS Approach to Unravel Preeclampsia NIH Grant R01HD084628 (PI – Irina Buhimschi) PI on the subcontract from University Illinois Chicago to pay salary for Maksim Kouza May 1, 2019 – May 31, 2020, \$67,608 total

The Research Institute at Nationwide Children’s Hospital 2019 Fall Trainee Travel Award, sept 1, 2019, Award of \$1,500 for Dr. Maksim Kouza to attend International Conference on Mathematical Multiscale Modeling in Biology, Guanacaste, Costa Rica, October 21-25, 2019.

The Research Institute at Nationwide Children’s Hospital Travel Award May 18, 2018, Award of \$1,500 for Dr. Maksim Kouza to attend Protein Society 2018 Annual Symposium in Boston, MA

Protein Sequence Matching: NIH Grant R01GM127701 (\$1,823,539.00 Apr 02, 2018- Apr 01, 2023) – PI (Multi-PI grant with Iowa State University)

Protein Sequence Matching: NIH Grant Supplement \$148,624 in 2018 to purchase computational infrastructure) – PI (Multi-PI grant with Iowa State University)

ABI Innovation: Collaborative Research: Computational Identification and Screening for Deleterious Mutants, NSF DBI 1661391 (\$883,059.00 Jun 01, 2017 to May 31, 2020) - with Iowa State University

High-Accuracy Protein Models Derived from Lower Resolution Data, NIH Grant 5R01GM081680-03 (\$712,834 Sept 15, 2007 – Aug 31, 2011) – PI

High-Accuracy Protein Models Derived from Lower Resolution Data, NIH Grant 5R01GM081680-03S1 Administrative Supplement (\$52,007 Sept 30, 2007 – Aug 31, 2010) – PI

Coarse-Grained Models of Proteins, NIH Grant 2R01GM072014-05A1 (\$2,600,000 Jul 01 2004 –Dec 31 2013) – CoPI (with Robert L. Jernigan, PI)

Modeling Ribosomal Control, Function and Assembly, NIH Grant 5R01GM073095-04 (\$1,000,000 Sept 25, 2006 – Aug 31, 2011) – CoPI (with Robert L. Jernigan, PI)

Structural Interpretation of the Protein Interactome, NSF MCB 1021785 (\$582,006) Aug 01, 2010-July 31, 2014) CoPI (with Robert L. Jernigan, PI)

Improving Livestock Gene Annotations, Center of Animal Genomics, ISU Grant (\$100,000 Jul 01, 2007- Jun 30, 2009) – CoPI (with Robert L. Jernigan, PI)

Bibliography

Peer-reviewed papers in journals:

1. Stecki, J. and Kloczkowski, A.: Statistical Mechanics of Liquid-Crystalline Ordering. *Zfi Mitt.* 13: 104-111, 1978.
2. Stecki, J. and Kloczkowski, A.: On the Stability of the Orientational Distribution of Molecules. *J. de Physique (Paris) C3*: 360-362, 1979.
3. Stecki, J. and Kloczkowski, A.: On the Stability of the Isotropic Phase Towards Nematic and Smectic A Phase Formation. *Mol. Physics* 42: 51-63, 1981.
4. Kloczkowski, A. and Stecki, J.: On the Mean Spherical Model for Liquid Crystals. *Mol. Physics* 46: 13-19, 1982.
5. Kloczkowski, A. and Stecki, J.: Stability in the Mean Spherical Model for Hard Spheres with Dipole Moments. *Acta Physica Polonica A61*: 493-496, 1982.
6. Lipszyc, K. and Kloczkowski, A.: The Isotropic-Nematic Phase Transition as the Bifurcation of Solutions of the Nonlinear Integral Equation. *Acta Physica Polonica A63*: 805-822, 1983.
7. Frisch, H.L. and Kloczkowski, A.: A Simple Model for Protection Against Environmental Pollution in Reactive Coating Films. *J. Colloid Int. Sci.* 99: 404-419, 1984.
8. Escher, C., Kloczkowski, A. and Ross, J.: Increased Power Output and Resonance Effects in a Thermal Engine Driven by a Unimolecular or Bimolecular Model Reaction. *J. Chem. Phys.* 82: 2457-2565, 1985.
9. Kloczkowski, A. and Stecki, J.: A Molecular Model for the Smectic A Phase. *Mol. Physics* 55: 689-700, 1985.
10. Kloczkowski, A. and Stecki, J.: On the Tricritical Points in the McMillan Model of Liquid Crystals. *Mol. Physics* 55: 1223-1232, 1985.
11. Kloczkowski, A. and Luckhurst, G.R.: On the Relationship of the Nematic-Isotropic Transition Temperature of an Oligomer to that of Its Constituent Units. *Liquid Crystals* 3:95-99, 1988.
12. Kloczkowski, A. and Luckhurst, G.R.: Transition Temperatures of Binary Nematic Mixtures predicted by the Humphries-James-Luckhurst Theory. *J. Chem. Soc. Faraday Trans.* 84: 155-159, 1988.
13. Kloczkowski, A., Luckhurst, G.R. and Phippen, R.W.: A Visual Representation for the Shapes of Flexible Mesogenic Molecules. *Liquid Crystals* 3: 185-194, 1988.
14. Kloczkowski, A. and Samborski, A.: Freezing of the Hard Core Yukawa Fluid. *J. of Chem. Phys.* 88: 5834-5839, 1988.
15. Kloczkowski, A. and Samborski, A.: Quadrupoles on the Triangular Two-Dimensional Lattice: A Simple Model of N₂ on Graphite Herringbone Transition. *Langmuir* 4: 817- 821, 1988.

16. Kloczkowski, A., Mark, J.E. and Erman, B.: Chain Dimensions and Fluctuations in Random Elastomeric Networks I. Phantom Gaussian Networks in the Undeformed State. *Macromolecules* 22: 1423-1432, 1989.
17. Erman, B., Kloczkowski, A. and Mark, J.E.: Chain Dimensions and Fluctuations in Random Elastomeric Networks II. Dependence of Chain Dimensions and Fluctuations on Macroscopic Strain. *Macromolecules* 22: 1432-1437, 1989.
18. Kloczkowski, A. and Mark, J. E.: On the Pace-Datner Theory of Diffusion of Small Molecules Through Polymers. *J. Polym. Sci., Polym. Phys. Ed.* 27: 166-1674, 1989.
19. Samborski, A. and Kloczkowski, A.: Quadrupoles on the Triangular 2D Lattice. The Influence of the External Field of Graphite. *Langmuir* 5: 1071-1074, 1989.
20. Kloczkowski, A., Mark, J.E. and B. Erman: The Small Angle Neutron Scattering from Elastomeric Networks: I. Calculated Scattering from a Path Containing Several Junctions in the James-Guth Model. *Macromolecules* 22: 4502-4506, 1989.
21. Kloczkowski, A., Mark, J.E. and Erman, B.: Neutron Scattering from Elastomeric Networks: II. An Alternative Phantom Network Model. *Macromolecules* 23: 1222-1224, 1990.
22. Kloczkowski, A., Mark, J.E., Bahar, I. and Erman, B.: A Closed Form Solution for the Internal Dynamics of Polymer C chains. I. Bonds with Independent Rotational Potentials. *J. Chem. Phys.* 92: 4513-4518, 1990.
23. Kloczkowski, A., Mark, J.E., and H. L. Frisch, H.L.: Relaxation Spectrum for Gaussian Networks. *Macromolecules* 23: 3481-3490, 1990.
24. Kloczkowski, A., Mark, J.E. and Erman, B.: On the Flory-Ronca Theory of Systems of Rodlike Particles. *Macromolecules* 23: 5035-5037, 1990.
25. Erman, B., Bahar, I., Kloczkowski, A. and Mark, J.E.: A Lattice Model for Segmental Orientation in Deformed Polymeric Networks. I. Contribution of Intermolecular Correlations. *Macromolecules* 23: 5335-5340, 1990.
26. Erman, B., Bahar, I., Kloczkowski, A. and Mark, J.E.: A Lattice Model for Segmental Orientation in Deformed Polymeric Networks. II. Effect of Chain Stiffness and Thermotropic Interactions. *Macromolecules* 23: 5341-5346, 1990.
27. Kloczkowski, A., Mark, J.E. and Erman, B.: Fluctuations, Correlations and Small Angle Neutron Scattering from Endlinked Chains in Regular Bimodal Networks. *Macromolecules* 24: 3266-3275, 1991.
28. Kloczkowski, A., Mark, J.E., Erman, B. and Eichinger, B.E.: Comment on: "Statistical Mechanics of Rubber Elasticity." *J. Chem. Phys.* 95: 7015-7016, 1991.
29. Kloczkowski, A., Mark, J.E. and Erman, B.: Correlations Among Chains in a Crosslinked Path in a Phantom Network and Their Characterization by SANS. *Macromolecules* 25: 2455-2458, 1992.
30. Kloczkowski, A., Mark, J.E. and Erman, B.: Application of the James-Guth Model in Modern Theories of Neutron Scattering from Polymer Networks. *Comput. Polymer Sci.* 2: 8-31, 1992.
31. Sharaf, M.A., Kloczkowski, A., Mark, J.E. and Erman, B.: Networks Undergoing Strain Induced Crystallization. Analysis by the Constrained Junction Model. *Comput. Polymer Sci.* 2: 84, 1992.
32. Trohalaki, S., Kloczkowski, A., Mark, J.E., Roe, R.J. and Rigby, D.: Molecular Dynamics Simulation of Small-Molecule Diffusion in Polyethylene. *Comput. Polymer Sci.* 2: 147-151, 1992.

33. Kloczkowski, A., Sharaf, M.A. and Mark, J.E., Molecular Theory for Reinforcement in Filled Polymers. *Comput. Polymer Sci.* 3: 39-45, 1993.
34. Yang, Y., Kloczkowski, A., Mark, J.E., Erman, B. and Bahar, I.: A Novel Orientation Technique for Semi-Rigid Polymers. 1. Preparation of Cross-Linked Cellulose Acetate and Hydroxypropylcellulose Films Having the Required Permanent Anisotropy in the Swollen State. *Colloid Polymer Sci.* 272: 284-292, 1994.
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2. Yan, A., Kloczkowski, A., and Jernigan, R.L., Identifying the Structural Clusters and Outliners of Structural Families Using Several Clustering Methods.
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High Performance Biodegradable Materials from Oriented Starch Derivatives, J. E. Mark, B. Z. Paterson, B. Erman, I. Bahar, A. Kloczkowski, US Patent # 6,218,532 B1, April 17, 2001. The Reissue Patent Number US RE 38,773 E, August 9, 2005.

Synergetic Activities

Research

Statistical mechanics of protein folding. Prediction of protein structure and function. Statistical mechanics of elastomeric networks. Protein dynamics. Prediction of protein binding sites. Contact potentials in proteins. Prediction of post-translational modification sites in proteins.

Reviews

Frequent reviews for Proteins: Structure, Function, and Bioinformatics, Biophysical Journal, Protein Science, Bioinformatics, Chemical Biology & Drug Design, Journal of Chemical Physics, Journal of Biomolecular Screening, Macromolecules, Polymer, and many other journals. Grant reviewer for NSF, NIH, and Polish Science Foundation.

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