Prof. Pemra Doruker

Correspondance: Department of Chemical Engineering and Polymer Research Center Bogazici University, Bebek, 34342 Istanbul, TurkeyPhone: +90-212-358 7365 Fax: +90-212-2575032e-mail: doruker@boun.edu.tr http://klee.bme.boun.edu.tr/pemra Education:Ph.D. in Chemical Engineering, Bogazici University, Turkey, 1991-1995M.S. in Chemical Engineering, Bogazici University, Turkey, 1989-1991B.S. in Chemical Engineering, Bogazici University, Turkey, 1983-1987 Academic and Research Positions: Professor: June 2005- present. Chemical Engineering Department, Bogazici University, Istanbul, Turkey Associate Professor: Nov 1999-May 2005. Chemical Engineering Department, Bogazici University, Istanbul, Turkey (with tenure since Oct 2000) Assistant Professor: Feb 1999- Oct 2000. Chemical Engineering Department, Bogazici University, Istanbul, Turkey Postdoctoral Fellow: May 1996-Feb 1999. Wayne L. Mattice’s laboratory at the Institute of Polymer Science, University of Akron (OH), U.S.A. Oct 1995- May 1996. Burak Erman’s laboratory at Polymer Research Center, Bogazici University, Istanbul, Turkey. Research and Teaching Assistant: Feb 1990- July 1995. Chemical Engineering Department, Bogazici University, Turkey. Visiting Scientist: June 2005: Robert L. Jernigan’s laboratory, Baker Center for Bioinformatics and Biological Sciences at Iowa State University, Ames, Iowa, USA.July 2004: Lennart Nilsson’s laboratory at the Center for Structural Biochemistry, Karolinska Institute, Novum Research Park, Huddinge, SwedenJune-August 2002, July 2004: Lennart Nilsson’s laboratory at the Center for Structural Biochemistry, Karolinska Institute, Novum Research Park, Huddinge, SwedenJuly-August 2001: Robert L. Jernigan’s laboratory at the National Cancer Institute, Laboratory of Experimental and Computational Biology, National Institutes of Health, Bethesda (MD), USA August 2000: Robert L. Jernigan’s laboratory at the National Cancer Institute, Laboratory of Experimental and Computational Biology, National Institutes of Health, Bethesda (MD), USA. June 1999- Sep 1999. Wayne L. Mattice’s laboratory at the Institute of Polymer Science, University of Akron, Akron (OH), U.S.A. June 1995- Sep 1995. Wayne L. Mattice’s laboratory at the Institute of Polymer Science, University of Akron, Akron (OH), U.S.A. Awards: “2002 Young Scientist Award” given by TUBA (Turkish National Academy of Sciences)“2001 Young Scientist Encouragement Prize” given by TUBITAK (Turkish National Science and Technology Foundation) “Outstanding Achievement in Research Prize” given by the Bogazici University Research Foundation, Istanbul, 2001"1995 Ph.D. Thesis Award" given by Bogazici University Research Foundation, Istanbul Fellowships:EMBO (European Molecular Biology Organization) Short-term Fellowship, 2002TUBITAK Postdoctoral Fellow, 1995-1996TUBITAK Ph. D. Fellowship, 1993-1995 Publications (SCI Journals):1. Kurkcuoglu O., Jernigan R.L., Doruker P. “Loop motions of triosephosphate isomerase observed with elastic networks” Biochemistry 45, 1173-1182 (2006) 2. Alakent B., Camurdan M.C., Doruker P. “Hierarchical structure of the energy landscape of proteins revisited by time series analysis. I. Mimicking protein dynamics in different time scales” Journal of Chemical Physics 123, 144910 (2005)3. Alakent B., Camurdan M.C., Doruker P. “Hierarchical structure of the energy landscape of proteins revisited by time series analysis. II. Investigation of explicit solvent effects” Journal of Chemical Physics 123, 144911 (2005)4. Kantarci N., Tamerler C., Sarikaya M., Haliloglu T., and Doruker P. “Molecular dynamics simulations on constraint metal binding peptides” Polymer 46, 4307-4313 (2005)5. Kurkcuoglu, O.; Jernigan, R.L.; Doruker, P. “Collective dynamics of large proteins from mixed coarse-grained elastic network model” QSAR & Combinatorial Science 24, 443-448 (2005)6. Yildirim Y.; Doruker P. “Collective motions of RNA polymerases. Analysis of core enzyme, elongation complex and holoenzyme” Journal of Biomolecular structure & dynamics, 22, 267-280 (2004)7. Alakent B.; Doruker, P.; Camurdan, M.C. “Application of time series analysis on molecular dynamics simulations of proteins. A study on different conformational spaces by principal component analysis” Journal of Chemical Physics121, 4759-4769 (2004) 8. Kucukpinar, E.; Doruker, P. “Effect of absorbed water on oxygen transport in EVOH matrices.” Polymer 45, 3555-3564 (2004) 9. Kurkcuoglu, O.; Jernigan, R.L.; Doruker, P. “Mixed levels of coarse-graining of large proteins using elastic network model succeeds in extracting the slowest motions” Polymer 45, 649-657 (2004) 10. Alakent B.; Doruker, P.; Camurdan, M.C. “Time series analysis of collective motions in proteins” Journal of Chemical Physics 120, 1072-1088 (2004) 11. Doruker, P.; Jernigan, R.L. “Functional motions can be extracted from on-lattice construction of proteins” Proteins 53, 174-181 (2003) 12. Kucukpinar, E.; Doruker, P. “Molecular simulations of small gas diffusion and solubility in copolymers of styrene” Polymer 44, 3607-3620 (2003) 13. Doruker, P.; Jernigan, R. L.; Navizet, I.; Hernandez, R. “Important fluctuation dynamics of large protein structures are preserved upon coarse-grained renormalization.” International Journal of Quantum Chemistry 90, 822-837 (2002) 14. Isin, B.; Doruker, P.; Bahar, I. “Functional motions of influenza virus hemagglutinin: A structure-based analytical approach” Biophysical Journal 82, 569-581 (2002) 15. Doruker, P.; Bahar, I.; Baysal, C.; Erman, B. “Collective Deformations in Proteins Determined by a Mode Analysis of Molecular Dynamics Trajectories” Polymer 43, 431-439 (2002) 16. Doruker, P; Jernigan, R. L.; Bahar, I. “Dynamics of large protein systems through hierarchical levels of coarse-grained structures” Journal of Computational Chemistry 23, 119-127 (2002) 17. Doruker, P. “Simulation of Polyethylene Thin Films Composed of Various Chain Lengths” Polymer 43, 425-430 (2002) 18. Doruker P; Mattice WL "Effect of surface roughness on structure and dynamics in thin films" Macromolecular Theory and Simulations 10, 363-367 (2001) 19. Doruker, P.; Wang, Y.; Mattice, W.L. (2001) "Simulation of the Random Scission of C-C Bonds in the Initial Stage of Thermal Degradation of Polyethylene" Computational and Theoretical Polymer Science 11, 155-166. 20. Doruker, P.; Atilgan, A. R.; Bahar, I. (2000) "Dynamics of Proteins Predicted by Molecular Dynamics Simulations and Analytical Approaches: Application to alpha-Amylase Inhibitor" Proteins 40, 512-524. 21. Baschnagel, J.; Binder, K.; Doruker, P.; Gusev, A. A.; Hahn, O.; Kremer, K.; Mattice, W. L.; Müller-Plathe, F.; Murat, M.; Paul, W.; Santos, S.; Suter, U. W.; Tries, V. (2000) "Bridging the Gap between Atomistic and Coarse-Grained Models of Polymers: Status and Perspectives" Advances in Polymer

Science 152, 41-156. 22. Ozisik, R.; Doruker, P.; Mattice, W. L.; von Meerwall, E. D. (2000) "Translational Diffusion In Monte Carlo Simulations of Polymer Melts: Center of Displacement vs. Integrated Autocorrelation Function" Computational and Theoretical Polymer Science 10, 411-418. 23. Vao-soongnern, V.; Doruker, P.; Mattice, W.L. (2000) "Simulation of an Amorphous Polyethylene Nanofiber on a High Coordination Lattice" Macromolecular Theory and Simulations 8, 1-13.24. Doruker, P.; Mattice, W.L. (1999) "A Second Generation of Mapping/ Reverse Mapping of Coarse-Grained and Fully Atomistic Models of Polymer Melts" Macromolecular Theory and Simulations 8, 463-478. 25. Doruker, P.; Mattice, W.L. (1999) "Segregation of Chain Ends is a Weak Contributor to Increased Mobility at Free Polymer Surfaces" Journal of Physical Chemistry B 103, 178-183. 26. Doruker, P.; Mattice, W.L. (1999) "Mobility of the Surface and Interior of Thin Films Composed of Amorphous Polyethylene" Macromolecules 32, 194-198.27. Birol, G.; Doruker, P.; Kirdar, B.; Önsan, Z. I., Ülgen, K. (1998) “Mathematical Formulation of Ethanol Fermantation by Immobilized Saccharomyces cerevisiae” Process Biochemistry 33, 763-771. 28. Doruker, P.; Mattice, W.L. (1998) "Dynamics of Bulk Polyethylene on a High Coordination Lattice" Macromolecular Symposia 133, 47-70.29. Doruker, P.; Mattice, W.L. (1998) "Simulation of Polyethylene Thin Films on a High Coordination Lattice” Macromolecules 31, 1418-1426.30. Doruker, P.; Mattice, W.L. (1997) "Reverse-mapping of Coarse-Grained Conformations on the Second Nearest Neighbor Diamond Lattice back to the Continuous Space" Macromolecules 30, 5520-5526. 31. Doruker, P.; Bahar, I. (1997) "Role of Water on Unfolding Kinetics of Helical Peptides Studied by Molecular Dynamics Simulations" Biophysical Journal 72, 2445-2456. 32. Bahar, I.; Cho, J.; Doruker, P.; Erman, B.; Haliloglu, T.; Kim, E.-G.; Mattice, W.L.; Monnerie, L.; Rapold, R.F. (1997) "Three Approaches That May Permit More Efficient Simulation of the Dynamics of Atomistic Models of Polymers" Trends in Polymer Science 5, 155-160. 33. Doruker, P.; Rapold, R.F.; Mattice, W.L. (1996) "Rotational Isomeric State Models for Polyoxyethylene and Polythiaethylene on a High Coordination Lattice" Journal of Chemical Physics 104, 8742-8749. 34. Doruker, P.; Önsan, Z.I.; KÄ±rdar, B. (1995) "Ethanol Fermentation by Growing S. cerevisiae Cells Immobilized in Small Ca-alginate Beads" Turkish Journal of Chemistry 19, 37-42. 35. Doruker, P., Bahar, I. (1993) "Effect of Intrachain Constraints and Polymer-Solvent Interactions on Chain Statistics and Dynamics" Computational Polymer Science, 3, 87-99. 36. Bahar, I.; Badur, B.; Doruker, P. (1993) "Solvent Effect on Translational Diffusivity and Segmental Orientational Mobility of Polymers in Dilute Solution: A Molecular Dynamics Study" Journal of Chemical Physics, 99, 2235-2246. Book Chapter: Vao-soongnern, V.; Doruker, P.; Mattice, W. L. "Simulations of Thin Films and Fibers of Amorphous Polymers", In "Computational Studies, Nanotechnology, and Solution Thermodynamics of Polymer Systems", Dadmun, M. D.; Van Hook, W. A.; Noid, D. W.; Melnichenko, Y. B.; Sumpter, B. G., Eds., Kluwer Academic/Plenum Publishers, New York, 2001, pp 117-126. Published Abstracts: 1. Jernigan R.L., Doruker P., Wang Y.M., Kundu S. “Protein motions with an efficient coarse-grained approach”Abstracts of Papers of the American Chemical Society 227: U897-U897 012-COMP Part 1 (2004)2. Isin, B.; Bahar, I.; Doruker, P. “Collective motions of neutral and low pH forms of influenza virus hemagglutinin” Biochemistry-US 40, 40 (2001) 3. Isin, B.; Bahar, I.; Doruker, P. “Collective motions of neutral and low pH forms of influenza virus hemagglutinin” Abstracts of Papers of the American Chemical Society 222: 40-BIOL Part 1 (2001) 4. Doruker, P.; Mattice, W. L. “Effect of surface roughness on structure and dynamics in thin films” Abstracts of Papers of the American Chemical Society 220: 190-PMSE Part 2 (2000) 5. Doruker, P.; Mattice, W. L. “Effect of chain end segregation on the mobility of thin films” Abstracts of Papers of the American Chemical Society 218: 38-MACR Part 2 (1999) 6. Doruker, P.; Mattice, W. L. “Dynamics of polyethylene films on a high coordination lattice” Abstracts of Papers of the American Chemical Society 215: 198-PMSE Part 2 (1998) 7. Doruker, P.; Cho, J. H.; Mattice, W. L. “Mapping-reverse mapping between atomistic models and high coordination lattices for the simulation of amorphous polymers” 213: 328-COMP Part 1 (1997) Presentations at Meetings: 1. Kurkcuoglu, O.; Jernigan, R.L.; Doruker, P. “Mixed coarse-grained elastic network model analysis on triosephosphate isomerase”, VIth European Symposium of the Protein Society, Barcelona, 20052. Kantarci, N.; Doruker, P.; Haliloglu, T. “Vibrational and conformational dynamic analysis of p53 core domain” ”, VIth European Symposium of the Protein Society, Barcelona, 2005 3. Kurkcuoglu, O.; Jernigan, R.L.; Doruker, P. “A mixed coarse-graining study on triosephosphate isomerase” Chemical Physics VI, Yeditepe Üniversitesi, Ä°stanbul, 2004.4. Alakent, B.; Doruker, P.; Camurdan, M.C. “Investigation of collective motions in proteins by time series analysis” Chemical Physics VI, Yeditepe Üniversitesi, Ä°stanbul, 2004.5. Özen, A.S., Aviyente, V.; Doruker, P. “Azo-hydrazone tautomerism in azo dyes: A DFT study” Chemical Physics VI, Yeditepe Üniversitesi, Ä°stanbul, 2004.6. Kurkcuoglu, O.; Jernigan, R.L.; Doruker, P. “Collective dynamics of large proteins from mixed coarse-grained elastic network model” The 15th European Symposium on QSAR & Molecular Modelling, Istanbul, 2004.7. Kantarci, N.; Tamerler, C.; Sarikaya, M.; Haliloglu, T.; Doruker, P. “Molecular dynamics simulations on metal binding peptides” The 15th European Symposium on QSAR & Molecular Modelling, Istanbul, 2004.8. Kucukpinar, E.; Doruker, P. “Modelling of diffusion and solubility of small gases in copolymers” (in Turkish), 15th National Chemistry Congress, Istanbul, 2001.9. Doruker, P.; Keskin, O.; Bahar, I; Jernigan, R.L. “Calculation of protein motions with extremely coarse-grained models” 4th European Symposium of the Protein Society, Paris, France, 2001.10. Isin, B.; Doruker, P.; Bahar, I. “Relating the structure of influenza virus hemagglutinin to membrane fusion mechanism by a structure-based analytical approach” 4th European Symposium of the Protein Society, Paris, France, 2001.11. Isin, B.; Doruker, P.; Bahar, I. “Functional motions of influenza virus hemagglutinin: A Gaussian network model analysis”, 12th National Biophysical Congress, Istanbul, 2001.12. Doruker, P.; Bahar, I. “Molecular dynamics simulation of a-amylase inhibitor” ”, 12th National Biophysical Congress, Istanbul, 2001.13. Doruker, P.; Mattice, W.L. "Coarse-grained simulations on the stability of thin films" National Meeting of American Chemical Society, Washington, D.C., U.S.A., 2000.14. Doruker, P.; Mattice, W.L. "The Effect of Chain End Segregation on the Mobility of Thin Films" Symposium on Polymeric Materials in Separations-National Meeting of American Chemical Society, New Orleans (LA), U.S.A., 1999.15. Doruker, P.; Mattice, W.L.

"Dynamics of Polyethylene Films on a High Coordination Lattice "Symposium on Modelling of Polymers, National Meeting of American Chemical Society, Dallas, Texas, U.S.A., 1998.16. Doruker, P.; Mattice, W.L. "Dynamics of Polyethylene Thin Films" Molecular Modelling of Polymers- American Chemical Society, Isle of Palms (SC), U.S.A., 1998.17. Doruker, P.; Mattice, W.L. "Simulation of Polyethylene on a High Coordination Lattice" Mini-Symposium on Polymer Simulation- Highways and Byways, Department of Materials, Institute of Polymers, ETH, Zurich, Switzerland, 1997.18. Doruker, P.; Cho, J.; Mattice, W.L. " Mapping/ Reverse Mapping Between Atomistic Models and High Coordination Lattices for the Simulation of Amorphous Polyethylene" Symposium on Modelling of Polymers- National Meeting of American Chemical Society, San Francisco (CA), U.S.A., 1997.19. Doruker, P.; Mattice, W.L. "Simulation of Polymers Using Rotational Isomeric State Chains on High Coordination Lattices" American Institute of Chemical Engineers National Meeting, Chicago (IL), U.S.A., 1996.20. Doruker, P.; Mattice, W.L. "Successful Mapping of Rotational Isomeric Polyoxyethylene on a High Coordination Lattice" Mini-Symposium on Polymer Simulation- Highways and Byways, Max-Planck-Institut fur Polymerforschung and Institut fur Physik, Universitat Mainz, Mainz, Germany, 1996.21. Cho, J.; Doruker, P., Mattice, W.L. "Simulation of Bulk Polyethylene on the Second Nearest Neighbor Diamond Lattice" Workshop on Modeling of Industrial Materials: Connecting Atomistics and Quantum Scales, Institute of Theoretical Physics, University of California, Santa Barbara (CA), U.S.A., 1996.22. Doruker, P.; Bahar, I. "Simulation of Single Chains in Different Solvent Conditions" NATO-ASI on Frontiers of Chemical Dynamics, Kemer, Turkey, 1994.23. Doruker, P.; Bahar, I. "A Molecular Dynamics Study of the Intramolecular and Intermolecular Effects on the Scattering and Orientational Behavior of Polymers in Dilute Solution" NSF-TUBITAK Joint Workshop on Polymer Coil Collapse, Istanbul, Turkey, 1994.24. Doruker, P., Bahar, I., "The Effect of Polymer-Solvent Interactions on the Static and Dynamic Properties of Polymers" (in Turkish), 9th Chemistry and Chemical Engineering Symposium, Trabzon, Turkey, 1993.25. Doruker, P.; Bahar, I. "Solvent Effect on Local Chain Dynamics" 33rd Microsymposium on Optics and Dynamics of Polymers, Prag, Check Republic, 1993. 26. Doruker, P.; Bahar, I. "A Molecular Dynamics Study of Solvent Effect on Behavior of Bead-Spring Model Chains in Solution" Chemical Physics II, Bilkent Üniversitesi, Ankara, Turkey, 1993.27. Doruker, P., Z. Ä°. Önsan, B. KÄ±rdar, "The Immobilization Characteristics of High Ethanol Producing S. cerevisiae"(in Turkish), 7th Chemistry and Chemical Engineering Symposium, Gazi MaÄŸusa, Cyprus, 1991. Projects: § 2005-2009: 6th Framework Program, FP6-2004-ACC-SSA-2 Project on “Towards Excellence in Computational Structural Biology and Biomaterials (COSBIOM)”, Polymer Research Center (co-investigator)§ 2005-2009: TÜBÄ°TAK Proje on ‘Determination of Structure-Function Relationships of Biomolecular Systems by Efficient Simulation Techniques’ (PI)§ 2005-2008: DPT (Turkish State Planning Organization) Project on “Synthesis and Design of New Metal-binding Biomaterials” (PI)§ 2003-2004: BoÄŸaziçi University Research Project (03R104) on "Computational Grid for Modeling of Biological Systems and Polymeric Materials” (PI)§ 2003-2005: Bogazici University Research Project (03A501-D) on “Polypeptide-Metal Surface Interactions” (PI)§ 2001-2003: Bogazici University Research Fund Project (01HA501) on “Modeling of Barrier Properties of Polymeric Membranes” (PI)§ 1999-2001: Bogazici University Research Fund Project (99HA501) on "Protein-Membrane Interactions" (PI)§ 2001-2004: DPT Project on "Determination of Molecular Structure and Functions of Proteins and Biomolecular Complexes Using Bioinformatics Tools and Computer Simulations" (co-investigator)§ 1996-1998: Project “NSF DMR 9523278" on "Configuration and Dynamics of Large Polymeric Systems", director: W. L. Mattice (co-investigator)§ 1995: Project "NSF INT 9312285" on "Dynamics of Polymeric Systems", International Program, director: W. L. Mattice (co-investigator)