VLASIS G. MAVRANTZAS

OFFICE ADDRESS
ETH Zürich
Institut f. Verfahrenstechnik
ML F 14.2
Sonneggstrasse 3
8092 Zürich
e-mail: vlasiosm@mat.ethz.ch
vlasis@chemeng.upatras.gr
tel.: + 41 44 632 8503
mobile: +30 6944 60 25 80
+41 788 17 35 98

HOME ADDRESS
Lerchenberg 6
8046 Zürich
Switzerland
Tel.: +41 44 55 88 570

PERSONAL

Date of birth: January 4, 1966
Marital status: Married (with Vasiliki Mavrozoumi; have 1 son, George)
Citizenship: Greek
Languages: English, Greek, some German
Leisure activities: Literature and poetry reading, listening to radio, playing soccer

ACADEMIC INTERESTS

- Physical Chemistry, Chemical Engineering Thermodynamics, Statistical Thermodynamics, Non-equilibrium Thermodynamics
- Statistical Mechanics, Molecular Simulations
- Dynamics and Rheology of micro-structured fluids
- Finite-Element and Spectral-Element Numerical Methods

RESEARCH INTERESTS

- Modeling and simulation of polymers and of soft nanostructured polymeric materials at multiple time and length scales (atomistic, mesoscopic, macroscopic)
- Multiscale modeling of chain dynamics and rheology (viscoelasticity) in polymers as a function of the molecular architecture of the chains (linear, branched, rings)
- Modeling polymers at interfaces (adhesion, self-assembly, dynamics in confined geometries)
- Thermodynamics of complex fluids under non-equilibrium conditions
- Constitutive modeling of polymer viscoelasticity
- Molecular modelling and simulation of the phase state of atmospheric organic aerosol particles, and prediction of their physicochemical properties
- Quantum Field Theory

EDUCATION

Ph.D. in Chemical Engineering
University of Delaware, Newark, Delaware, April 1994
- *GPA*: 4.0/4.0
- *Dissertation*: "Surface effects on the conformation and rheology of polymer solutions"
- *Advisor*: Prof. A.N. Beris
- *Minor*: Mathematics and Physics (GPA: 4.0/4.0)

Diploma in Chemical Engineering
National Technical University (NTU), Athens, Greece, July 1988
- *GPA*: 9.24/10.00 (top 1%)
- *Diploma thesis*: "Regional energy planning in the islands of the Cyclades complex"
- *Advisor*: Prof. M. Koukios

PROFESSIONAL EXPERIENCE

Dozent-Lecturer (September 2016- today)
Department of Mechanical and Process Engineering (with Prof. S.E. Pratsinis), Particle Technology Laboratory, ETH Zürich, Switzerland

Guest Professor (September 2014- September 2016)
Department of Mechanical and Process Engineering (with Prof. S.E. Pratsinis), Particle Technology Laboratory, ETH Zürich, Switzerland

Guest Professor (September 2013- August 2014)
Department of Materials Science (with Prof. Hans Christian Öttnger), Institute of Polymers, ETH Zürich, Switzerland

Professor (July 2011-today)
Department of Chemical Engineering, University of Patras, Patras, Greece

Associate Professor (July 2003-July 2011)
Department of Chemical Engineering, University of Patras, Patras, Greece

Researcher B' (November 2001-July 2003)
Institute of Chemical Engineering and High-Temperature Chemical Processes, ICE/HT-FORTH, Patras, Greece

Researcher C' (October 1997-October 2001)
Institute of Chemical Engineering and High-Temperature Chemical Processes, FORTH-ICE/HT, Patras, Greece

Post-Doctoral Research Assistant (January 1996-October 1997)
Institute of Chemical Engineering and High-Temperature Chemical Processes and Department of Chemical Engineering, University of Patras, Patras, Greece

Military Service (May 1994-December 1995)
War Material Corps, Didymoteicho, Evros, and Army Chemistry Labs, Piraeus, Greece

Ph.D. Research Assistant (September 1989-April 1994)
Department of Chemical Engineering, University of Delaware, USA

OTHER PROFESSIONAL ACTIVITIES

Visiting Scientist

- Institute of Polymers, Department of Materials, ETH-Zürich, Switzerland (January-February 2013, June-July 2012, February 2006, February 2002, February 2000, with Prof. Hans Christian Öttinger)
- Technical University of Denmark (DTU), Lyngby, Denmark (June-July 2010, with Prof. George Kontogeorgis)
- Norwegian University of Science and Technology (NTNU), Trondheim, Norway (February 2010, with Prof. Zhiliang Zhang)
- Department of Applied Physics, University of Tokyo, Japan (June-July 2005, with Prof. Masao Doi)
- Dow Chemical Company, Midland, USA (December 2000, with Dr. Joey Storer)
- University of Delaware, Department of Chemical Engineering, Newark, DE, USA (August 1999, with Prof. Antony Beris)

Collaborating Faculty Member

- Inter-Departmental Programme of Graduate Studies in "Polymer Science and Technology", University of Patras (1999-today)
- Department of Materials Science, University of Patras (2000-2002)

National Delegate

- In the Working Party on Thermodynamics and Transport Properties (WP-TTP), one of the seventeen WPs of the European Federation of Chemical Engineering (EFCE)

HONORS

- On the International Advisory Board of the Journal: *Macromolecular Theory and Simulation*, Wiley-VCH, Germany, since 2005
- President of the Hellenic Society of Rheology (HSR), September 2004-to date
- Director, Inter-department Programme of Graduate Studies on "Polymer Science and Technology", University of Patras, 2003-to date
- The Allan P. Colburn Prize in Engineering and Mathematical Sciences, for the PhD thesis dissertation titled: "Surface Effects on the Structure and the Rheology of Dilute Polymer Solutions", University of Delaware, 1993-1994
- University of Delaware Competitive Fellowship, 1991-1992
- Thomaidis Excellence Award for graduating first in class of 1988, NTUA
- Economou Excellence Award for graduating first in class of 1988, NTUA
- Technical Chamber of Greece Excellence Award for graduating first in class of 1988, NTUA
- Outstanding Undergraduate Student Excellence Awards, annually 1983-1988, NTUA

PROFESSIONAL AFFILIATIONS

- Member, American Institute of Chemical Engineers (AIChE)
- Member, American Physical Society (APS)
- Member, Society of Rheology (SOR)
- Member, Polymer Processing Society (PPS)
- Member, Technical Chamber of Greece (TEE)
- Secretary, Hellenic Society of Rheology (HSR)

PARTICIPATION IN RESEARCH AND DEVELOPMENT PROJECTS

NATO CRG 1998 [1]

- NATO collaborative research grant titled: *From the Rouse to the Entangled Polymer Melt Regime*
- Contract No: CRG.CRG.973023
- Partners: FORH-ICE/HT, Univ. of Delaware (USA)
- Budget: 216 kBEF
- Contribution to the Lab: 216 kBEF
- Duration: 1998-2000
- Project Coordinator: V.G. Mavrantzas

GeMColloidS [2]

- EC research project (MARIE-CURIE Host Development Fellowship) titled: *Generic Methodologies in Colloids and Suspensions*
- Contract No: HPMD-CT-2000-00054
- Partners: FORTH-ICE/HT
- Total EC contribution: 228 kEuro
- EC contribution to the Lab: 228 kEuro
- Duration: 2001-2004
- Project coordinator: V.G. Mavrantzas

NATO CRG 2001 [3]

- NATO collaborative linkage grant titled: *Structure and Dynamics in Crystalline Polymers: Vibrational Spectroscopy and Molecular Simulation*
- Contract No: CRG.CRG.973023

- Partners: FORH-ICE/HT, MIT, University of Jerusalem
- Total budget: 8,000 USD
- Contribution to the Lab: 8,000 USD
- Duration: 2001-2003
- Project Coordinator: V.G. Mavrantzas

PMILS [4]

- EC Growth research project titled: *Polymer Modeling at Integrated Length/Time Scales*
- Contract No: G5RD-CT-2002-00720
- Partners: UPM (Coordinator), FORTH-ICE/HT, Borealis, Rhodia, NKT, DTU, Imperial College, CPERI, Namur, Ip-Sol
- Total EC contribution: 2,689 kEuro
- EC contribution to the Lab: 423.1 kEuro
- Duration: 2002-2005
- Project Coordinator: Manolo Laso
- Research leader from FORTH-ICE/HT: V.G. Mavrantzas

PROSMAK [5]:

- GSRT PENED 2001 project titled: *The role of grafted macromolecules to the stability of nanoparticles (applications to the technology of paintings)*
- Code: 01ED587
- partners: FORTH-ICE/HT (coordinator), University of Patras, FORTH-IESL, INTERCHEM-HELLAS
- Total budget: 220 kEuro
- Contribution to the Lab: 50 kEuro
- Duration: 2002-2005
- Project Coordinator: V.G. Mavrantzas

ESOPO [6]

- GSRT PENED 2001 project titled: *Study of the effects of mechanical stress and temperature in the extrusion of reinforced polyethylene pipes*
- Code: 01ED136
- Partners: FORTH-ICE/HT (coordinator), University of Patras, Petzetakis SA
- Total budget: 193.7 kEuro
- Contribution to the Lab: 46 kEuro
- Duration: 2002-2005
- Project Coordinator: V. Gregoriou

Dow Chemicals Industrial Project I [7]

- Industrial research project with Dow Benelux B.V. titled: *Multi-scale simulation of polyethylene melt rheological and processing properties*
- Contract No: Research contract with the Dow Chemical Company (USA and The Netherlands)
- Partners: FORTH-ICE/HT (coordinator), Dow Benelux (Netherlands)
- Total budget: 86.4 kUSD
- Contribution to the Lab: 86.4 kUSD
- Duration: 2002-2005
- Project coordinator: V.G. Mavrantzas

AKMON 2004 [8]

- GSRT project titled: *Design and characterization of heterogeneous materials for applications in the technologies of energy and environment*

- Partners: FORTH-ICE/HT (coordinator), University of Patras
- Total budget: 481 kEuro
- Contribution to the Lab: 106 kEuro
- Duration: 2004-2007
- Project coordinator: V. Burganos

Karatheodori 2004 [9]

- University of Patras project titled: *Prediction of the structural and interfacial properties of aqueous solutions of n-alkyl poly(oxy ethyl ethers) from molecular simulations*
- Partners: University of Patras
- Total budget: 40.5 kEURO
- Contribution to the Lab: 23.5 kEuro
- Duration: 2004-2007
- Project coordinator: V.G. Mavrantzas

Pythagoras II 2004 [10]

- Ministry of Education of Greece project titled: *New numerical techniques for the computation of flows of viscoelastic materials under conditions of industrial applications*
- Partners: University of Patras
- Total budget: 50 kEuro
- Contribution to the Lab: 25 kEuro
- Duration: 2005-2007
- Project coordinator: J. Tsamopoulos

DOW Chemicals Industrial project II [11]

- Industrial research project with Dow Benelux B.V. titled: *Multi-scale simulation of polyethylene melt rheology and processing properties*
- Contract No: Research contract with Dow Chemical Company (USA)
- Partners: FORTH-ICE/HT (coordinator), Dow Benelux (Netherlands), Dow Chemical Company (USA)
- Total budget: 75 kEuro
- Contribution to the Lab: 75 kEuro
- Duration: 2006-2008
- Project coordinator: V.G. Mavrantzas

DYNACOP [12]

- EC research project (FP7-PEOPLE-2007-1-1-ITN) titled: *Dynamics of complex polymers*
- Contract No: DYNACOP
- Partners: ULeeds (coordinator), FORTH, FZJ, Univ. del Pais, UTwente, UCL, DTU, UNaples, DOW, UAthens
- Total EC contribution: ~3,000 kEuro
- EC contribution to the Lab: 70 kEuro
- Duration: 2009-2012
- Project coordinator: T.C.B. Mcleish
- Project leader from FORTH: D. Vlassopoulos

MODIFY [13]

- EC (FP7-NMP-2008-SMALL-2) project titled: *Multi-scale modeling of interfacial phenomena in acrylic adhesives undergoing deformation*
- Contract No: 228320
- Partners: Univ. of Patras (coordinator), ESPCI, CNRS, UCL, ETH-Z, DOW, LBI
- Total EC contribution: 2,863 kEuro

- EC contribution to the Lab: 402.3 kEuro
- Duration: 2009-2012
- Project coordinator: V.G. Mavrantzas

HERACLITUS [14]

- National project titled: *Molecular mechanisms governing slip phenomena during the flow of polymeric melts past solid substrates*
- Partners: UPatras
- Total National contribution: 45 kEuro
- National contribution to the Lab: 45 kEuro
- Duration: 2010-2013
- Project coordinator: V.G. Mavrantzas

PEPPER [15]

- EC (FP7-ENERGY-2009-TREN-2) project titled: *Demonstration of high performance processes and equipments for thin film silicon photovoltaic modules produced with lower environmental impact and reduced cost and material use*
- Contract No: 249782
- Partners: OS (coordinator), IMT, UPatras, UoN, ETF, HSPH, Linde
- Total EC contribution: 9,380 kEuro
- EC contribution to the Lab: 60 kEuro
- Duration: 2010-2013
- Project coordinator: Tobias Roschek
- Project leader from the University of Patras: D. Mataras

BioNexGen [16]

- EC (FP7-NMP-2009-SMALL-3) project titled: *Development of the next generation membrane bioreactor system*
- Contract No: 246039
- Partners: HSKA (Coordinator), CNR-ITM, UON, FORTH, SEZ, MN, IZTECH, ABU, CMRDI, CBS, NTX
- Total EC contribution: 3,420 kEuro
- EC contribution to the Lab: 60 kEuro
- Duration: 2010-2013
- Project coordinator: Jan Hoinkis
- Project leader from FORTH-ICE/HT: G. Vogiatzis

MMM@HPC [17]

- EC (FP7-INFRA-2010-1.2.2) project titled: *Multiscale materials modeling on high performance computing*
- Partners: KIT (Coordinator),CSC-IT, UPatras, UMons, CEA Grenoble, CINECA Bologna, Li-Tec Battery, BASF, Nokia, Sony
- Total EC contribution: 2,800 kEuro
- EC contribution to the Lab: 214 kEuro
- Duration: 2011-2013
- Project coordinator: Wolfgang Wenzel
- Project leader from the University of Patras: V.G. Mavrantzas

MEKKA [18]

- National project (synergasia) titled: *Development of carbon nanotube based polymeric membranes for industrial wastewater treatment and water reuse*
- Contract No: 620-11/11/2009

- Partners: FORTH-ICE/HT, UPatras, INTERCHEM
- Total National Contribution: 425 kEuro
- EC contribution to the Lab: 80 kEuro
- Duration: 2011-2013
- Project coordinator: V.G. Mavrantzas

THALES [19]

- National project (Thales) titled: *Graphene and its nanocomposites: Production, properties and applications*
- Partners: FORTH-ICE/HT
- Total National Contribution: 400 kEuro
- Contribution to the Lab: 30 kEuro
- Duration: 2012-2015
- Project coordinator: C. Galiotis

ARISTEIA 2011 [20]

- National project (Aristeia 2011) titled: *General method for the simulation of self-organization in nanostructured polymeric systems*
- Partners: Univ. of Patras
- Total National Contribution: 300 kEuro
- Contribution to the Lab: 300 kEuro
- Duration: 2012-2015
- Project coordinator: V.G. Mavrantzas

BioSmartTrainee [21]

- EC research project (H2020-MSCA-ITN-2014) titled: *Training in Bio-Inspired Design of Smart Adhesive Materials (BioSmartTrainee)*
- Contract No: DYNACOP
- Partners: LIFP-Dresden (coordinator), MPI-P, WU, ESPCI, BASF, Cambridge Univ., TUE, UPatras, AkzoNobel, URGO
- Total EC contribution: ~ 2,822 kEuro
- EC contribution to the Lab: 221 kEuro
- Duration: 2015-2018
- Project coordinator: Alla Synytska (LIFP-Dresden)
- Project leader from UPatras: V.G. Mavrantzas

Limmat [22]

- Limmat Foundation donation project (MuSiComPS) titled: *Multiscale Simulations of Complex Polymer Systems (MuSiComPS)*
- Contract No: MuSiComPS
- Partners: NTUA, UPatras
- Total Limmat Foundation contribution: ~668 kEuro
- Contribution to the Lab: 179 kEuro
- Duration: 2015-2018
- Project coordinator: D.N. Theodorou
- Project leaders from UPatras: V.G. Mavrantzas, J. Tsamopoulos

FORCE [23]

- EC research project (H2020-NMBP-2016-2017) titled: *Formulations and Computational Engineering (FORCE)*
- Contract No: FORCE
- Partners: Dow, Unilever UK, IBM-Zurich, Fraunhofer IWM/ITWM, Enthought Ltd.,

EnginSoft Spa, Granta Design Ltd., UPatras, Megara Resins S.A., ETH-Z

- Total EC contribution: ~ 5,417 kEuro
- EC contribution to the Lab in Patras: 294.1 kEuro
- EC contribution to the Lab in Zurich: 478.5 kEuro
- Duration: 2016-2020
- Project coordinator: Adham Hashibon (Fraunhofer IWM/ITWM)
- Project leader from UPatras: V.G. Mavrantzas

PUBLICATIONS IN REFEREED JOURNALS (* denotes corresponding author)

1. **V.G. Mavrantzas**, A.N. Beris,* "Theoretical study of wall effects on the rheology of dilute polymer solutions", *J. Rheol.* **1992**, *36*, 175-213.
2. **V.G. Mavrantzas**, A.N. Beris,* "Modeling the rheology and flow-induced concentration changes in polymer solutions", *Phys. Rev. Lett.* **1992**, *69*, 273-276.
3. **V.G. Mavrantzas**, A. Souvaliotis, A.N. Beris,* "Pseudospectral calculations of stress-induced concentration changes in simple viscometric flows of polymer solutions", *Theoret. Comput. Fluid Dynam.* **1993**, *5*, 3-31.
4. A.N. Beris,* **V.G. Mavrantzas**, "On the compatibility between various macroscopic formalisms for the concentration and flow of dilute polymer solutions", *J. Rheol.* **1995**, *38*, 1235-1250.
5. B.J. Edwards, A.N. Beris,* **V.G. Mavrantzas**, "A model with two coupled Maxwell modes", *J. Rheol.* **1996**, *40*, 917-942.
6. **V.G. Mavrantzas,** D.N. Theodorou,* "Atomistic simulation of polymer melt elasticity: Free energy calculation of an oriented polymer melt", *Macromolecules* **1998**, *31*, 6310-6332.
7. V.A. Harmandaris, **V.G. Mavrantzas**, D.N. Theodorou,* "Atomistic molecular dynamics simulations of polydisperse linear polyethylene melts", *Macromolecules* **1998**, *31*, 7934-7943.
8. **V.G. Mavrantzas**, A.N. Beris,* "A hierarchical model for surface effects on chain conformation and rheology of polymer solutions: A) General formulation", *J. Chem. Phys.* **1999**, *110*, 616-627.
9. **V.G. Mavrantzas**, A.N. Beris,* "A hierarchical model for surface effects on chain conformation and rheology of polymer solutions: B) Application to a neutral surface", *J. Chem. Phys.* **1999**, *110*, 628-638.
10. **V.G. Mavrantzas**, T. Boone, E. Zervopoulou, D.N. Theodorou,* "End-bridging Monte Carlo: A fast algorithm for atomistic simulation of condensed phases of long polymer chains", *Macromolecules* **1999**, *32*, 5072-5096.
11. V.A. Harmandaris, **V.G. Mavrantzas**, D.N. Theodorou,* "Atomistic molecular dynamics simulations of stress relaxation upon cessation of steady-state uniaxial elongational flow", *Macromolecules* **2000**, *33*, 8062-8076.
12. **V.G. Mavrantzas**, D.N. Theodorou,* "Atomistic Monte Carlo simulation of the elasticity of long-chain polyethylene melts: Dependence of chain degree of orientation on stress, molecular weight, and rate of elongation", *Macromol. Theory Simul.* **2000**, *9*, 500-515. (Invited paper for special issue in honor of Prof. Oscar Friedrich Olaj).
13. **V.G. Mavrantzas**, D.N. Theodorou,* "Atomistic simulation of the birefringence of uniaxially stretched polyethylene melts", *Comput. Theor. Polymer Sci.* **2000**, *10*, 1-13. (Invited paper for special issue in honor of Prof. Ueli Suter).
14. N.Ch. Karayiannis, **V.G. Mavrantzas**, D.N. Theodorou,* "Diffusion of small molecules in disordered media: study of the effect of kinetic and spatial heterogeneities", *Chem. Eng. Sci*. **2001**, *56*, 2789-2801.
15. E. Zervopoulou, **V.G. Mavrantzas**, D.N. Theodorou,* "A new Monte Carlo simulation approach for the prediction of sorption equilibria of oligomers in polymer melts: Solubility of long alkanes in linear polyethylene", *J. Chem. Phys.* **2001**, *115*, 2860-2875.
16. I.-E. Mavrantza, D. Prentzas, **V.G. Mavrantzas**,* C. Galiotis, "Detailed atomistic Molecular Dynamics simulation of the orthorhombic phase of polyethylene crystals and n-alkane paraffins with the COMPASS force field", *J. Chem. Phys*. **2001**, *115*, 3937-3950.
17. A. Uhlherr,* **V.G. Mavrantzas**, M. Doxastakis, D.N. Theodorou, "Directed bridging methods for fast atomistic Monte Carlo simulations of bulk polymers", *Macromolecules* **2001**, *34*, 8554-8568.
18. M. Doxastakis, **V.G. Mavrantzas**, D.N. Theodorou,* "Atomistic Monte Carlo simulation of cis-

1,4 polyisoprene melts. I. Single temperature end-bridging Monte Carlo simulations", *J. Chem. Phys*. **2001**, *115*, 11339-11351.

19. M. Doxastakis, **V.G. Mavrantzas**, D.N. Theodorou,* "Atomistic Monte Carlo simulation of cis-1,4 polyisoprene melts. II. Parallel-tempering end-bridging Monte Carlo simulations", *J. Chem. Phys*. **2001**, *115*, 11352-11361.
20. V.A. Harmandaris, M. Doxastakis, **V.G. Mavrantzas**,* D.N. Theodorou, "Detailed molecular dynamics simulation of the self-diffusion of n-alkane and cis-1,4 polyisoprene oligomer melts", *J. Chem. Phys*. **2002**, *116*, 436-446.
21. **V.G. Mavrantzas**,* H.C. Öttinger, "Atomistic Monte Carlo simulation of polymer melt elasticity: their nonequilibrium thermodynamics GENERIC formulation in a canonical ensemble", *Macromolecules* **2002**, *35*, 960-975.
22. M.V. Apostolakis, **V.G. Mavrantzas**,* A.N. Beris, "Stress gradient-induced migration effects in the Taylor-Couette flow of a dilute polymer solution", *J. Non-Newt. Fluid Mech.* **2002,** *102*, 409-445. (Invited paper for special issue in honor of Prof. Andreas Acrivos).
23. A. Uhlherr,* M. Doxastakis, **V.G. Mavrantzas**, D.N. Theodorou, S.J. Leak, N.E. Adam, P.E. Nyberg, "Atomic structure of a high polymer melt", *Europhys. Lett.* **2002**, *57*, 506-511.
24. N. Ch. Karayiannis, **V.G. Mavrantzas**,* D.N. Theodorou, "A novel Monte Carlo scheme for the rapid equilibration of atomistic model polymer systems of precisely defined molecular architecture", *Phys. Rev. Lett*. **2002**, *88*, 105503-1 105503-4.
25. A. Uhlherr,* S.J. Leak, N. Adam, P.E. Nyberg, M. Doxastakis, **V.G. Mavrantzas**, D.N. Theodorou, "Parallel, domain decomposition Monte Carlo for the fast simulation of large-scale bulk polymers", *Comp. Phys. Commun.* **2002**, *144*, 1-22.
26. V.A. Harmandaris, D. Angelopoulou, **V.G. Mavrantzas**, D.N. Theodorou,* "Atomistic molecular dynamics simulation of diffusion in binary n-alkane/polyethylene melts", *J. Chem. Phys*. **2002**, *116*, 7656-7665.
27. K.Ch. Daoulas, A.F. Terzis, **V.G. Mavrantzas**,* "Detailed atomistic Monte Carlo simulation of grafted polymer melts: I. Conformational and thermodynamic properties", *J. Chem. Phys*. **2002**, *116*, 11028-11038.
28. N. Ch. Karayiannis, A.E. Giannousaki, **V.G. Mavrantzas**,* D.N. Theodorou, "Atomistic Monte Carlo simulation of strictly monodisperse long polyethylene melts through a generalized chain bridging algorithm", *J. Chem. Phys.* **2002**, *117*, 5465-5479.
29. K.Ch. Daoulas, **V.G. Mavrantzas**,* D.J. Photinos, "Detailed atomistic Monte Carlo simulation of grafted polymer melts: II. Structural properties and NMR spectra", *J. Chem. Phys*. **2002**, *118*, 1521-1532.
30. N. Ch. Karayiannis, A.E. Giannousaki, **V.G. Mavrantzas**,* "An advanced Monte Carlo method for the equilibration of model long-chain branched polymers with a well-defined molecular architecture: Detailed atomistic simulation of an H-shaped polyethylene melt", *J. Chem. Phys.* **2003**, *118*, 2451-2454.
31. V.A. Harmandaris, **V.G. Mavrantzas**,* D.N. Theodorou, M. Kröger, J. Ramírez, H.C. Öttinger, D. Vlassopoulos, "Crossover from Rouse to entangled polymer melt regime: Signals from long, detailed atomistic molecular dynamics simulations, supported by rheological experiments", *Macromolecules* **2003**, *36*, 1376-1387.
32. K.Ch. Daoulas, A.F. Terzis, **V.G. Mavrantzas**,* "Variable connectivity methods for the atomistic Monte Carlo simulation of inhomogeneous and/or anisotropic polymer systems of precisely defined chain length distribution: Tuning the spectrum of chain relative chemical potentials", *Macromolecules* **2003**, *36*, 6674-6682.
33. A. Eilmes,* R.W. Munn, **V.G. Mavrantzas**, D.N. Theodorou, A. Góra, "Microscopic calculation of the static electric susceptibility of polyethylene", *J. Chem. Phys.* **2003**, 119, 11458-11466.
34. N.Ch. Karayiannis, **V.G. Mavrantzas,** D.N. Theodorou,* "Detailed atomistic simulation of the segmental dynamics and barrier properties of amorphous poly(ethylene terephthalate) and poly(ethylene isophthalate)", *Macromolecules* **2004**, *37*, 2978-2995.
35. K. Foteinopoulou, **V.G. Mavrantzas,*** J. Tsamopoulos, "Numerical simulation of bubble growth in Newtonian and viscoelastic filaments undergoing stretching", *J. Non-Newt. Fluid Mech*. **2004,** *122*, 177-200.
36. G. Tsolou, **V.G. Mavrantzas,*** D.N. Theodorou, "Detailed atomistic molecular dynamics

simulation of *cis*-1,4-poly(butadiene)", *Macromolecules* **2005**, *38*, 1478-1492.

37. K.Ch. Daoulas, V.A. Harmandaris, **V.G. Mavrantzas**,* "Detailed atomistic simulation of a polymer melt/solid interface: Structure, density and conformation of a thin film of polyethylene melt adsorbed on graphite", *Macromolecules* **2005**, 38, 5780-5795.
38. V.A. Harmandaris, K.Ch. Daoulas, **V.G. Mavrantzas**,* "Molecular dynamics simulation of a polymer melt/solid interface: Local dynamics and chain mobility in a thin film of polyethylene melt adsorbed on graphite", *Macromolecules* **2005**, 38, 5796-5809.
39. K.Ch. Daoulas, D.N. Theodorou,* V.A. Harmandaris, N.Ch. Karayiannis, **V.G. Mavrantzas**, "Self-consistent-field study of compressible semiflexible melts adsorbed on a solid substrate and comparison with atomistic simulations", *Macromolecules* **2005**, 38, 7134-7149.
40. N.Ch. Karayiannis, **V.G. Mavrantzas,*** "Hierarchical modelling of the dynamics of polymers with a non-linear molecular architecture: Calculation of branch point friction and chain reptation time of H-shaped polyethylene melts from long molecular dynamics simulations", *Macromolecules* **2005**, 38, 8583-8596.
41. **V.G. Mavrantzas**,* A.N. Beris, F. Leermakers, G. Fleer, "Continuum formulation of the Scheutjens-Fleer lattice statistical theory for homopolymer adsorption from solution", *J. Chem. Phys.* **2005**, 123, 174901-174915.
42. G. Tsolou, V.A. Harmandaris, **V.G. Mavrantzas**,* "Atomistic molecular dynamics simulation of the temperature and pressure dependence of local and terminal relaxation in *cis*-1,4-polybutadiene", *J. Chem. Phys.* **2006**, *124*, 084906.
43. K. Foteinopoulou, **V.G. Mavrantzas**,*Y. Dimakopoulos, J. Tsamopoulos, "Numerical simulation of multiple bubbles growing in a Newtonian liquid filament undergoing stretching", *Phys. of Fluids* **2006**, *18*, 042106.
44. G. Tsolou, V.A. Harmandaris, **V.G. Mavrantzas**,* "Local structure and chain packing in *cis*-1,4-polybutadiene systems: Detailed atomistic molecular dynamics simulation of their temperature and pressure dependence", *Macromolecular Theory & Simulations* **2006**, *15*, 381-393.
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   Chapter 7: Coarse-graining
   Chapter 8: Entanglement network-based simulations of deformation and flow
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PRESENTATIONS (speaker underlined)

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4. **V.G. Mavrantzas**, A.N. Beris, "Modeling and simulation of the dilute polymer solution flow behavior next to solid surfaces and interfaces", *National Meeting of the American Chemical Society*, San Francisco, April 5-10, **1992**.
5. **V.G. Mavrantzas**, A.N. Beris, "Interfacial phenomena in the rheology of dilute polymer solutions", *AIChE Annual Meeting*, Miami Beach, November 1-6, **1992**.
6. A.N. Beris, **V.G. Mavrantzas**, "Non-local effects in polymer rheology: Polymer-surface interactions", *Society of Rheology Meeting*, Boston, October 17-21, **1993**.
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27. I.E. Mavrantza, D. Prentzas, **V.G. Mavrantzas**, C. Galiotis, "Detailed atomistic molecular dynamics simulation of the temperature dependence of the IR vibrational spectra of crystalline polyethylene", *2nd Seminar of the Greek Network of Polymers*, Patras, April 6, **2001**.
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152. P.S. Stephanou, **V.G. Mavrantzas**, "Improved tube models for the dynamics of entangled polymer melts", Proceedings, *FLOW 2012 Meeting*, Volos, Greece, November 16-17, **2012**.
153. P.S. Stephanou, **V.G. Mavrantzas**, G.C. Georgiou, "A constitutive equation for the description of the rheological behavior of polymer nanocomposites based on principles of non-equilibrium thermodynamics", Proceedings, *FLOW 2012 Meeting*, Volos, Greece, November 16-17, **2012**.
154. **V.G. Mavrantzas**, T. Koukoulas, D. Tsalikis, P.S. Stephanou, "Atomistic molecular dynamics simulations of the conformational, dynamic, and topological properties of ring polymer melts", *245th ACS National Meeting & Exposition*, New Orleans, USA, April 7-11, **2013**.
155. P.S. Stephanou, **V.G. Mavrantzas**, G.C. Georgiou, "A constitutive equation for the description of the rheological behavior of polymer nanocomposites based on principles of non-equilibrium thermodynamics", *9th Panhellenic Chemical Engineers Conference*, Athens, Greece, 23-25 May, **2013**.
156. P.S. Stephanou, **V.G. Mavrantzas**, "Modeling at multiple scales of the linear viscoelastic properties of polymer melts: From atoms, to molecules, to primitive paths, to tube models", *9th Panhellenic Chemical Engineers Conference*, Athens, Greece, 23-25 May, **2013**.
157. E. Skountzos, A. Anastassiou, S. Sabethai, **V.G. Mavrantzas**, D.N. Theodorou, "Polymer-graphene nanocomposites: atomistic modeling and simulation of their mechanical properties", *9th Panhellenic Chemical Engineers Conference*, Athens, Greece, 23-25 May, **2013**.
158. T. Koukoulas, D. Tsalikis, P.S. Stephanou, **V.G. Mavrantzas**, "Conformational dynamics and topological analysis for polymer rings via atomistic molecular-dynamics simulations and comparison with experimental data", *10th HSTAM International Congress on Mechanics*, Chania, Crete, Greece, 25-27 May, **2013**.
159. E. Karahaliou, A. Anastasiou, **V.G. Mavrantzas**, "Water permeability through CNT-polymer nanocomposites: an atomistic simulation study", *10th HSTAM International Congress on Mechanics*, Chania, Crete, Greece, 25-27 May, **2013**.
160. A. Anastassiou, **V.G. Mavrantzas**, "Molecular dynamics simulation of the adhesive properties of acrylic polymers", *10th HSTAM International Congress on Mechanics*, Chania, Crete, Greece, 25-27 May, **2013**.
161. O. Alexiadis, **V.G. Mavrantzas**, "All-atom molecular dynamics simulation of the structural, thermodynamic, and packing properties of the pure amorphous and pure crystalline phases of regioregular P3HT", *6th International Symposium on Flexible Organic Electronics (ISFOE13)*, Thessaloniki, Greece, 8-11 July, **2013.**
162. P.S. Stephanou, **V.G. Mavrantzas**, G.C. Georgiou, "A differential constitutive equation for polymer nanocomposites based on principles of non-equilibrium thermodynamic", *Thermodynamics 2013*, Manchester, UK, September 3-6, **2013**.

163. **V.G. Mavrantzas**, P.S. Stephanou, C. Baig, "Multiscale modeling of entangled polymers: from atoms, to primitive paths, to tube models, to the linear viscoelasticity of high-MW polymer melts", *246th ACS National Meeting & Exposition, Indianapolis*, USA, September 8-12, **2013**.
164. P.V. Alatas, **V.G. Mavrantzas**, "Applications of a Thermodynamic, Non-Linear Quantum Master Equation to a Three-Level and a Harmonic Oscillator System Coupled with Two Heat Baths", *29th Panhellenic Conference on Solid State Physics and Materials Science*, Athens, Greece, September 22-25, **2013**.
165. P.S. Stephanou, **V.G. Mavrantzas**, G.C. Georgiou, "A differential constitutive equation for polymer nanocomposites based on principles of non-equilibrium thermodynamics", *9th Annual European Rheology Conference (AERC-2014)*, Karlsruhe, Germany, April 8-11, **2014**.
166. P.S. Stephanou, **V.G. Mavrantzas**, "Multi-scale modeling of high-MW polymer melt viscoelasticity starting from the atomistic level", *9th Annual European Rheology Conference (AERC-2014)*, Karlsruhe, Germany, April 8-11, **2014**.
167. D.G. Tsalikis, T. Koukoulas, **V.G. Mavrantzas**, "Conformational dynamics and topological analysis of polymer rings via atomistic molecular dynamics simulations and comparison with experimental data", *9th Annual European Rheology Conference (AERC-2014)*, Karlsruhe, Germany, April 8-11, **2014**.
168. E. Skountzos, A. Anastassiou, **V.G. Mavrantzas**, "Atomistic modeling and simulation of the dynamic and mechanical properties of poly(methyl methacrylate) - graphene nanocomposites", *7th International Meeting of the Hellenic Society of Rheology (HSR 2014)*, Heraklion, Crete, Greece, June 07-10, **2014.**
169. D.G. Tsalikis, **V.G. Mavrantzas**, "Threading of ring poly(ethylene oxide) molecules by linear chains in the melt under equilibrium and non-equilibrium molecular dynamics simulations", *7th International Meeting of the Hellenic Society of Rheology (HSR 2014)*, Heraklion, Crete, Greece, June 07-10, **2014.**
170. P.S. Stephanou, **V.G. Mavrantzas**, G.C. Georgiou, "A non-equilibrium thermodynamics-based model for the phase behavior, microstructure and rheology of polymer nanocomposite melts", *7th International Meeting of the Hellenic Society of Rheology (HSR 2014)*, Heraklion, Crete, Greece, June 07-10, **2014.**
171. P.S. Stephanou, **V.G. Mavrantzas**, G.C. Georgiou, "Continuum Model for the Phase Behavior, Microstructure, and Rheology of Unentangled Polymer Nanocomposite Melts", *10th Hellenic Polymer Society Conference (ELEP 2014)*, Patras, Greece, December 04-06, **2014**.
172. D.G. Tsalikis, T. Koukoulas, **V.G. Mavrantzas**, D. Vlassopoulos, "Dynamic, conformational and topological properties of ring poly(ethylene oxide) melts from molecular dynamics simulations", *10th Hellenic Polymer Society Conference (ELEP 2014)*, Patras, Greece, December 04-06, **2014**.
173. F.D. Tsourtou, O. Alexiadis, **V.G. Mavrantzas**, V. Kolonias, E. Housos, "Atomistic Monte Carlo and Molecular Dynamics simulation of the bulk phase self-assembly of semifluorinated alkanes", *10th Hellenic Polymer Society Conference (ELEP 2014)*, Patras, Greece, December 04-06, **2014**.
174. P.G. Mermigkis, D.G. Tsalikis, **V.G. Mavrantzas**, "Prediction of the effective diffusivity of water inside CNT-based PMMA membranes, *10th Hellenic Polymer Society Conference (ELEP 2014)*, Patras, Greece, December 04-06, **2014**.
175. E. Skountzos, A. Anastassiou, **V.G. Mavrantzas**, D.N. Theodorou, "Determination of the mechanical properties of a poly(methyl methacrylate) nanocomposite with functionalized graphene sheets through detailed atomistic simulations", *10th Hellenic Polymer Society Conference (ELEP 2014)*, Patras, Greece, December 04-06, **2014**.
176. E.N. Skountzos, O. Alexiadis, K. Kasidiaris, **V.G. Mavrantzas**, "All-atom molecular dynamics simulation of the structural, thermodynamic, and packing properties of the pure amorphous and pure crystalline phases of P3HT and PQT semiconducting polymers", *4th International Conference on Multifunctional, Hybrid and Nanomaterials*, Sitges (near Barcelona), Spain, March 9-13, **2015**.
177. S Tsouka, Y. Dimakopoulos, **V.G. Mavrantzas**, J. Tsamopoulos, "Application of the DCR tube model in thin film flow of dilute entangled polymer solutions that exhibit flow-induced concentration changes", *10th Annual European Rheology Conference (AERC-2015)*, Nantes,

France, April 14-17, **2015**.

178. K.D. Papadimitriou, E.N. Skountzos, S. Gkermpoura, **V.G. Mavrantzas**, C. Galiotis, C. Tsitsilianis, "Synthesis and atomistic simulation of pyrene functionalized α,ω-PMMA as dispersing agent of graphene for the fabrication of polymer nanocomposites", *Frontiers in Polymer Science (POLY 2015)*, Riva del Garda, Italy, May 20-22, **2015**.
179. E.N. Skountzos, O. Alexiadis, C. Kasidiaris, **V.G. Mavrantzas**, "All-atom molecular dynamics simulation of the structural, thermodynamic, and packing properties of the pure amorphous and pure crystalline phases of P3HT and PQT semiconducting polymers", *Europolymer Conference on Conducting Polymeric Materials (EUPOC 2015)*, Gargnano, Lago di Garda, Italy, May 24-28, **2015**.
180. K. Karadima, **V.G. Mavrantzas**, S.N. Pandis, "Atmospheric Nanoparticles: A Molecular Dynamics Simulation Study", *1st Workshop of Graduates and Post-Docs in Chemical Engineering Sciences*, Patras, Greece, May 27, **2015**.
181. F.D. Tsourtou, O. Alexiadis, **V.G. Mavrantzas**, V. Kolonias, E. Housos, "Atomistic Monte Carlo and Molecular Dynamics simulation of the bulk phase self-assembly of semifluorinated alkanes", *1st Workshop of Graduates and Post-Docs in Chemical Engineering Sciences*, Patras, Greece, May 27, **2015**.
182. P.V. Alatas, **V.G. Mavrantzas**, H.C. Öttinger, "A non-linear thermodynamic master equation for open quantum systems and application to the phenomenon of electromagnetically induced transparency", *10th Panhellenic Chemical Engineers Conference*, Patras, Greece, June 4-6, **2015**.
183. K.S. Karadima, **V.G. Mavrantzas**, S.N. Pandis, "A molecular dynamics simulation study of atmospheric nanoparticles", *10th Panhellenic Chemical Engineers Conference*, Patras, Greece, 4-6 June, **2015**.
184. P.G. Mermigkis, D.G. Tsalikis, **V.G. Mavrantzas**, "Prediction of the effective diffusivity of water inside CNT-based PMMA membranes, *10th Panhellenic Chemical Engineers Conference*, Patras, Greece, June 4-6, **2015**.
185. F.D. Tsourtou, O. Alexiadis, **V.G. Mavrantzas**, V. Kolonias, E. Housos, "Atomistic simulation of the bulk phase self-assembly of semifluorinated alkanes", *10th Panhellenic Chemical Engineers Conference*, Patras, Greece, June 4-6, **2015**.
186. E.N. Skountzos, **V.G. Mavrantzas**, C. Tsitsilianis, "PMMA/Graphene nanocomposites: Atomistic simulation to predict graphene fine dispersability in polymer composites with the aid of functional PMMA", *10th Panhellenic Chemical Engineers Conference*, Patras, Greece, June 4-6, **2015**.
187. K.S. Karadima, **V.G. Mavrantzas**, S.N. Pandis, "A molecular dynamics simulation study of atmospheric nanoparticles", *28th European Symposium on Applied Thermodynamics (ESAT 2015)*, Athens, Greece, June 11-14, **2015**.
188. P.V. Alatas, **V.G. Mavrantzas**, "Applications of a thermodynamic, non-linear quantum master equation to a three-level and a harmonic oscillator system coupled with two heat baths", *28th European Symposium on Applied Thermodynamics (ESAT 2015)*, Athens, Greece, June 11-14, **2015**.
189. F.D. Tsourtou, O. Alexiadis, **V.G. Mavrantzas**, V. Kolonias, E. Housos, "Atomistic simulation of the bulk phase self-assembly of semifluorinated alkanes", *28th European Symposium on Applied Thermodynamics (ESAT 2015)*, Athens, Greece, June 11-14, **2015**.
190. E.N. Skountzos, O. Alexiadis, K. Kasidiaris, **V.G. Mavrantzas**, "Atomistic simulation of the structural and thermodynamic properties of organic semiconducting polymers", *28th European Symposium on Applied Thermodynamics (ESAT 2015)*, Athens, Greece, June 11-14, **2015**.
191. C. Baig, **V.G. Mavrantzas**, "Simulation of polymer melts beyond equilibrium using a non-dynamic method (GENERIC Monte Carlo) in an expanded ensemble", *7th International Workshop on Non-equilibrium Thermodynamics and Complex Fluids (IWNET 2015)*, Hilvarenbeek, The Netherlands, July 6-10, **2015**.
192. P. Stephanou, **V.G. Mavrantzas**, G.C. Georgiou, "A differential constitutive equation for polymer nanocomposites based on principles of non-equilibrium thermodynamics", *7th International Workshop on Non-equilibrium Thermodynamics and Complex Fluids (IWNET 2015)*, Hilvarenbeek, The Netherlands, July 6-10, **2015**.
193. D.G. Tsalikis, **V.G. Mavrantzas**, D. Vlassopoulos, "Structural, conformational, dynamic and topological properties of ring poly(ethylene oxide) melts from molecular dynamics simulations

and compasrion with experimental data", *8th GRACM International Congress on Computational Mechanics,* Volos, Greece, July 12-15 **2015**.

194. E.N. Skountzos, **V.G. Mavrantzas**, C. Tsitsilianis, "Atomistic simulation of pyrene functionalized α,ω-PMMA as dispersing agent of graphene for the fabrication of polymer nanocomposites", *8th GRACM International Congress on Computational Mechanics,* Volos, Greece, July 12-15 **2015**.
195. P.G. Mermigkis, D.G. Tsalikis, **V.G. Mavrantzas**, "Prediction of the effective diffusivity of water inside CNT-based PMMA membranes, *8th GRACM International Congress on Computational Mechanics,* Volos, Greece, July 12-15 **2015**.
196. P.S. Stephanou, I.Ch. Tsimouri, **V.G. Mavrantzas**, "Flow-induced orientation and stretching of entangled polymers in the framework of non-equilibrium thermodynamics", *20th Anniversary Meeting of the European Society of Rheology*, ETH-Zurich, Switzerland, March 31 - April 1, **2016**.
197. D.G. Tsalikis, **V.G. Mavrantzas**, "Topological constraints in polymer rings", *PRACE Scientific and Industrial Conference (PRACE Days16),* Budapest, Hungary, May 10-12, **2016**.
198. F. Tsourtou, **V.G. Mavrantzas**, "Optimized Atomistic Monte Carlo and Molecular Dynamics Algorithms for simulating self-assembly in soft matter", *PRACE Scientific and Industrial Conference (PRACE Days16),* Budapest, Hungary, May 10-12, **2016**.
199. E.N. Skountzos, **V.G. Mavrantzas**, "Large-scale atomistic Molecular Dynamics simulation study of polymergraphene nanocomposites", *PRACE Scientific and Industrial Conference (PRACE Days16),* Budapest, Hungary, May 10-12, **2016**.
200. V. Vasilev, E.N. Skountzos, E. Goudeli, **V.G. Mavrantzas**, S.E. Pratsinis, "Predicting the fractal-like structure of SiO2 nanoparticles through molecular dynamics simulations using the potential of mean force", *MaP Graduate Symposium*, ETH-Zurich, Switzerland, June 9, **2016**.
201. D.G. Tsalikis, **V.G. Mavrantzas**, D. Vlassopoulos, "Geometric analysis of ring-ring threading events in melts of ring polymers and their connection with the slow relaxation modes*", XVIIth International Congress on Rheology (ICR 2016),* Kyoto, Japan, August 8 - 13, **2016**.
202. P. Alatas, D. Tsalikis, **V.G. Mavrantzas**, "Molecular dynamics simulation of the structure and self-diffusion of short linear and cyclic n-alkanes in melt and blends", *2nd Workshop of Graduates and Post-Docs in Chemical Engineering Sciences*, Patras, Greece, September 23, **2016**.
203. P.S. Stephanou, D.G. Tsalikis, **V.G. Mavrantzas**, "Multiscale modelling approach to the rheological behavior of polymer nanocomposites: Nonequilibrium thermodynamics modeling coupled with NEMD simulations", *8th International Conference on Multiscale Materials Modeling (MMM-2016),* Dijon, France, October 9-14, **2016**.
204. P.V. Alatas, D. G. Tsalikis, **V.G. Mavrantzas**, "Comparison of the conformational and dynamic properties between ring and linear poly(ethylene oxide) melts from molecular dynamics simulations in the crossover regime from unentangled to entangled", *11th Hellenic Polymer Society Conference (ELEP 2016),* Heraklion, Crete, Greece, November 3-5, **2016**.
205. P.G. Mermigkis, E.N. Skountzos, **V.G. Mavrantzas**, "Atomistic molecular dynamics simulation of water mobility inside Carbon Nanotubes embedded in a PMMA matrix", *11th Hellenic Polymer Society Conference (ELEP 2016),* Heraklion, Crete, Greece, November 3-5, **2016**.
206. E.N. Skountzos, **V.G. Mavrantzas**, C. Tsitsilianis, "Atomistic simulation of pyrene functionalized α,ω-PMMA as dispersing agent of graphene for the fabrication of polymer nanocomposites", *11th Hellenic Polymer Society Conference (ELEP 2016),* Heraklion, Crete, Greece, November 3-5, **2016**.
207. P.S. Stephanou, D.G. Tsalikis, P.V. Alatas, **V.G. Mavrantzas**, "Non-equilibrium thermodynamics modelling and atomistic simulation of polymer nanocomposites", *11th Hellenic Polymer Society Conference (ELEP 2016),* Heraklion, Crete, Greece, November 3-5, **2016**.
208. D.G. Tsalikis, **V.G. Mavrantzas**, D. Vlassopoulos, "Geometric analysis of threading events in melts of ring polymers and their connection with the slow relaxation modes", *11th Hellenic Polymer Society Conference (ELEP 2016),* Heraklion, Crete, Greece, November 3-5, **2016**.
209. I.Ch. Tsimouri, Ch.K. Georgantopoulos, P.S. Stephanou, **V.G. Mavrantzas**, "Derivation of a recently proposed CCR model through the use of non-equilibrium thermodynamics", *11th Hellenic Polymer Society Conference (ELEP 2016),* Heraklion, Crete, Greece, November 3-5, **2016**.
210. F.D. Tsourtou, **V.G. Mavrantzas**, "Atomistic Monte Carlo and Molecular Dynamics Algorithms

for the simulation of self-assembly in soft matter", *11th Hellenic Polymer Society Conference (ELEP 2016)*, Heraklion, Crete, Greece, November 3-5, **2016**.

211. E.N. Skountzos, **V.G. Mavrantzas**, S.E. Pratsinis, "From atoms to primary particles to agglomerates: Hierarchical modeling of the fractal dimensions of nanoparticles", *2016 MRS Fall Meeting & Exhibit*, Boston, USA, November 27 - December 2, **2016**.
212. E.N. Skountzos, **V.G. Mavrantzas**, C. Tsitsilianis, "Atomistic simulation of pyrene functionalized α,ω-PMMA as dispersing agent of graphene for the fabrication of polymer nanocomposites", *2016 MRS Fall Meeting & Exhibit*, Boston, USA, November 27 - December 2, **2016**.
213. D.G. Tsalikis, E.N. Skountzos, **V.G. Mavrantzas**, "Computational study of microscopic dynamics in Polyethylene Glycol melts filled with Silica Nanoparticles and comparison with experimental data", *2016 MRS Fall Meeting & Exhibit*, Boston, USA, November 27 - December 2, **2016**.
214. P.S. Stephanou, D.G. Tsalikis, P.V. Alatas, **V.G. Mavrantzas**, "Multiscale modelling approach to the rheological behaviour of polymer nanocomposites: Nonequilibrium thermodynamics modelling coupled with NEMD simulations", *11th Annual European Rheology Conference (AERC-2017)*, Copenhagen, Denmark, April 3-6, **2017**.
215. I.Ch. Tsimouri, C.K. Georgantopoulos, P.S. Stephanou, **V.G. Mavrantzas**, "Derivation of a recently proposed CCR model through the use of non-equilibrium thermodynamics", *11th Annual European Rheology Conference (AERC-2017)*, Copenhagen, Denmark, April 3-6, **2017**.
216. D.G. Tsalikis, G.D. Papadopoulos, **V.G. Mavrantzas**, "Microscopic dynamics and topology of polymer rings immersed in a host matrix of longer linear polymers: Results from a detailed molecular dynamics simulation study and comparison with experimental data", *PRACE Scientific and Industrial Conference (PRACEdays17)*, Barcelona, Spain, May 16-18, **2017**.
217. F. Tsourtou, **V.G. Mavrantzas**, "Optimized Monte Carlo and Molecular Dynamics algorithms for modelling the self-organization of two classes of materials: semifluorinated alkanes and semiconducting polymers based on thiophenes", *PRACE Scientific and Industrial Conference (PRACEdays17)*, Barcelona, Spain, May 16-18, **2017**.
218. E.N. Skountzos, **V.G. Mavrantzas**, "Atomistic simulation of pyrene functionalized α,ω-PMMA as dispersing agent of graphene for the fabrication of polymer nanocomposites", *PRACE Scientific and Industrial Conference (PRACEdays17)*, Barcelona, Spain, May 16-18, **2017**.
219. P.V. Alatas, D.G. Tsalikis, **V.G. Mavrantzas**, "Molecular dynamics simulation of the differences in the conformational and dynamic properties between and linear polyethylene oxide melts in the crossover region from unentangled to entangled", *11th Panhellenic Chemical Engineers Conference*, Salonica, Greece, May 25-27, **2017.**
220. A. Spyrogianni, K.K. Karadima, E. Goudeli, **V.G. Mavrantzas**, S.E. Pratsinis, "Brownian dynamic simulation of the settling rate of fractal-like nanoparticle agglomerates", *11th Panhellenic Chemical Engineers Conference*, Salonica, Greece, May 25-27, **2017.**
221. D. Mallios, D.G. Tsalikis, **V.G. Mavrantzas**, "Self-assembly of amphiphile peptides into nanostructures through detailed molecular dynamics simulations", *11th Panhellenic Chemical Engineers Conference*, Salonica, Greece, May 25-27, **2017.**
222. P. Mermigkis, E.N. Skountzos, **V.G. Mavrantzas**, "Study of water molecule mobility in carbon nanotubes embedded in a PMMA matrix", *11th Panhellenic Chemical Engineers Conference*, Salonica, Greece, May 25-27, **2017.**
223. D. Mintis, P.V. Alatas, D.G. Tsalikis, **V.G. Mavrantzas**, "Conformational transition of poly(ethylene-imine) in aqueous solution at different protonation states and its role in the formation of complex coacervate elucidated from Atomistic Molecular Dynamics Simulations", *11th Panhellenic Chemical Engineers Conference*, Salonica, Greece, May 25-27, **2017.**
224. C.K. Georgantopoulos, I.Ch. Tsimouri, P.S. Stephanou, **V.G. Mavrantzas**, "Development of state-of-the-art constitutive rheological models for entangled polymeric fluids using principles of nonequilibrium thermodynamics",*11th Panhellenic Chemical Engineers Conference*, Salonica, Greece, May 25-27, **2017.**
225. E.N. Skountzos, D.G. Tsalikis, **V.G. Mavrantzas**, "On the effect of end-functionalized groups on the dynamics of polymer melt nanocomposites through molecular dynamics simulations", *11th Panhellenic Chemical Engineers Conference*, Salonica, Greece, May 25-27, **2017.**

226. P.S. Stephanou, D.G. Tsalikis, E.N. Skountzos, **V.G. Mavrantzas**, "Modelling of polymer nanocomposite melts based on principles of nonequilibrium thermodynamics and on the findings of detailed nonequilibrium molecular dynamics simulations", *11th Panhellenic Chemical Engineers Conference*, Salonica, Greece, May 25-27, **2017.**
227. I.Ch. Tsimouri, P.S. Stephanou, **V.G. Mavrantzas**, "A constitutive rheological model for the blodod from nonequilibrium thermodynamics", *11th Panhellenic Chemical Engineers Conference*, Salonica, Greece, May 25-27, **2017.**
228. F.D. Tsourtou, **V.G. Mavrantzas**, "Atomistic Monte Carlo and Molecular Dynamics simulation of nanostructured semiconducting polymers and polypeptides", *11th Panhellenic Chemical Engineers Conference*, Salonica, Greece, May 25-27, **2017.**
229. E.N. Skountzos, D.G. Tsalikis, **V.G. Mavrantzas**, "Molecular simulation of PMMA-graphene and PEO-silica polymer nanocomposites in full atomistic detail", *SCIMEETING Europe, Materials Modellig and Simulations Conference*, Athens, Greece, June 21-23, **2017**.
230. F. Tsourtou, S. Peroukidis, and **G. Mavrantzas**, "Monte Carlo and Molecular Dynamics simulation of liquid-crystalline phases of oligothiophenes using a united-atom model", *14th European Conference on Liquid Crystals (ECLC 2017)*, Moscow, Russia, June 24-30, **2017**.
231. K.S. Karadima, **V.G. Mavrantzas**, S.N. Pandis, "The effect of organics and humidity on the structure of atmospheric nanoparticles: A molecular dynamics simulation study", *20th International Conference on Nucleation and Atmospheric Aerosols (ICNAA 2017)*, Helsinki, Norway, June 25-39, **2017**.
232. P.S. Stephanou, D.G. Tsalikis, E.N. Skountzos, **V.G. Mavrantzas**, "Multiscale modelling approach to the rheological behaviour of polymer nanocomposites: Nonequilibrium thermodynamics modelling coupled with NEMD simulations", *8th International Meeting of the Hellenic Society of Rheology (HSR 2017)*, Limassol, Cyprus, July 12-14, **2017.**
233. D.G. Tsalikis, P.V. Alatas, **V.G. Mavrantzas**, "Ring polymers: scaling laws and topological interactions based on detailed molecular dynamics simulations", *8th International Meeting of the Hellenic Society of Rheology (HSR 2017)*, Limassol, Cyprus, July 12-14, **2017.**
234. P.S. Stephanou, **V.G. Mavrantzas**, "Multi-scale modelling of high-MW polymer melt viscoelasticity starting from the atomistic level", *8th International Meeting of the Hellenic Society of Rheology (HSR 2017)*, Limassol, Cyprus, July 12-14, **2017.**
235. I.Ch. Tsimouri, C.K. Georgantopoulos, P.S. Stephanou, **V.G. Mavrantzas**, "Derivation of a recently proposed CCR model through the use of non-equilibrium thermodynamics", *8th International Meeting of the Hellenic Society of Rheology (HSR 2017)*, Limassol, Cyprus, July 12-14, **2017.**
236. K.S. Karadima, **V.G. Mavrantzas**, S.N. Pandis, "Molecular dynamics simulation of atmospheric nanoparticles: local structure and morphology", *European Aerosol Conference (EAC 2017)*, Zurich, Switzerland, August 27-September 01, **2017**.
237. D.G. Tsalikis, **V.G. Mavrantzas**, "Microscopic dynamics and topology of polymer rings immersed in a host matrix of longer linear polymers: Results from a detailed molecular dynamics simulation study and comparison with experimental data", *Ring Polymers: Focused Workshop*, Heraklion, Crete, September 25-27, **2017**.
238. A. Spyrogianni, K.S. Karadima, E. Goudeli, **V.G. Mavrantzas**, S.E. Pratsinis, "Mobility and Sedimentation of Agglomerates with Polydisperse Primary Particles", *2017 Conference of the Americal Association for Aerosol Research (2017 AAAR)*, Raleigh, North Carolina, October 16-20, **2017**.
239. A. Spyrogianni, K.S. Karadima, E. Goudeli, **V.G. Mavrantzas**, S.E. Pratsinis, "Sedimentation of Agglomerates Consisting of Polydisperse Nanoparticles", *AIChE Annual Meeting*, Minneapolis, USA, October 29 - November 03, **2017**.
240. A. Spyrogianni, K.S. Karadima, E. Goudeli, **V.G. Mavrantzas**, S.E. Pratsinis, "Settling rate of agglomerates consisting of polydisperse primary particles by Brownian Dynamics", *AIChE Annual Meeting*, Minneapolis, USA, October 29 - November 03, **2017**.
241. D.G. Tsalikis, **V.G. Mavrantzas**, "Melt rheology of ring poly(ethylene oxide) melts and comparison with experimental data", *12th Annual European Rheology Conference (AERC-2018)*, Sorrento, Italy, April 17-20, **2018**.
242. **V.G. Mavrantzas**, P.V. Alatas, H.C. Öttinger, "Third-order perturbation expansion of the two-

point correlation function of the dissipative quantum φ^4 theory", *8th International Workshop on Non-equilibrium Thermodynamics and Complex Fluids (IWNET 2018),* Sint-Michielsgestel, The Netherlands, July 1-6, **2018**.

243. D. Mintis, **V.G. Mavrantzas**, "Atomistic molecular dynamics simulation of weak polyelectrolytes in water", *12th International Symposium on Polyelectrolytes (ISP2018),* Wageningen, The Netherlands, August 26-31, **2018**.
244. F.D. Tsourtou, K. Kardima, **V.G. Mavrantzas**, "Atomistic Monte Carlo: A powerful technique for simulating self-assembly in polypeptides", *BioExcel 2nd SIG Meeting: "Advanced Simulations for Biomolecular Research" @ ECCB 2018,* Athens, Greece, September 8, **2018**.
245. T.S. Alexiou, D.G. Tsalikis, P.V. Alatas, **V.G. Mavrantzas**, "Conformational and dynamic properties of DNA minicircles in aqueous solution from atomistic molecular dynamics simulations", *12th Hellenic Polymer Society International Conferemce (ELEP 2018),* Ioannina, Greece, September 30-October 3, **2018**.
246. P.G. Mermigkis, E.N. Skountzos, **V.G. Mavrantzas**, "Conformational, dynamic, and permeability properties of atactic poly(methyl methacrylate) - carbon nanotube (PMMA-CNT) nanocomposites from molecular simulations", *12th Hellenic Polymer Society International Conferemce (ELEP 2018),* Ioannina, Greece, September 30-October 3, **2018**.
247. D.G. Tsalikis, **V.G. Mavrantzas**, "Conformation and dynamics of ring polymers in dilute solutions of linear matrices: Results from a systematic molecular dynamics simulation study and comparison with experimental data", *12th Hellenic Polymer Society International Conferemce (ELEP 2018),* Ioannina, Greece, September 30-October 3, **2018**.

INVITED LECTURES

1. "*Atomistic simulation of the viscoelasticity of unentangled polymer melts*", Institute for Polymers, Department of Materials, ETH, Zürich, Switzerland, February **2000**.
2. "*Modeling the rheology of polymer melts through multiscale modeling*", Dow Chemicals, Midland, December **2000**.
3. "*Hierarchical modeling of the rheology of polymer melts*", CECAM-SIMU Workshop, Multiscale Modeling of Materials, Heraklion, Crete, July **2001**.
4. *"Atomistic simulation of polymer melts off equilibrium using principles of irreversible thermodynamics"*, CPERI-CERTH, Salonica, October **2001**.
5. *"Molecular simulations of polymers with emphasis on their viscoelasticity*", 5th Panhellenic Conference on Polymers, Heraklion, Crete, December 15-17, **2001**.
6. *"A hierarchical model for the rheology of polymers in confined geometries",* Institute for Polymers, Department of Materials, ETH, Zürich, Switzerland, February **2002**.
7. "*Polymer melts grafted on a solid substrate or graphite: Detailed atomistic simulation of their interfacial properties and ^{2}H-NMR spectrum*", XVIII Panhellenic Conference on Solid State Physics-Materials Science, Heraklion, Crete, September 15-18, **2002**.
8. "*Atomistic simulations of polymers at multiple time and length scales*", Max-Planck Institute for Polymer Research (MPI-P), Mainz, Germany, March **2003**.
9. "*Hierarchical modelling of polymers with a non-linear molecular architecture: Calculation of branch point friction and chain reptation time of an H-shaped polyethylene melt from detailed atomistic simulations*", 1st Mainz Materials Simulation Days (MMSD 2005), Max-Planck Institute for Polymer Research (MPI-P), Mainz, Germany, June 8-10, **2005**.
10. "*Hierarchical modelling of polymers with a non-linear molecular architecture: Calculation of branch point friction and chain reptation time of an H-shaped polyethylene melt from detailed atomistic simulations*", Japan Society of Technology (JST) Symposium: "Towards Multi-scale Modeling in Soft Matter", Tokyo, Japan, June 21-22, **2005**.
11. *Multi-scale modelling of polymers with a non-linear molecular architecture*", Keynote lecture, International Workshop on Mesoscale and Multiscale Description of Complex Fluids, Prato, Italy, July 5-8, **2006**.
12. "*Simulation of polymers with a non-linear molecular architecture*", ΕΚΕΤΑ-ΙΤΧΗΔ, February 3, **2006**.
13. "*Multi-scale modeling of polymers with a non-linear molecular architecture*", Keynote lecture, International Workshop on Mesoscale and Multiscale Description of Complex Fluids, Prato, Italy,

July 5-8, **2006**.

14. *"Thermodynamically guided atomistic Monte Carlo simulation of polymer melts beyond equilibrium",* International Workshop on Multi-scale Modeling and Simulation of Complex Fluids, Maryland, USA, April 13-19, **2007.**
15. *"Polymer melt viscoelasticity: What can we learn from molecular simulations",* Department of Materials Science, University of Crete, Heraklion, Crete, May 25, **2007**.
16. *"Polymer melt viscoelasticity: What can we learn from molecular simulations",* Department of Applied Physics, University of Eindhoven, Eindhoven, The Netherlands, October 1, **2007**.
17. *"Hierarchical Modeling of Polymers: From the atomistic to the meso- to the macro-scale",*ENPC, Paris, November 26, **2007**.
18. *"Modeling in nanomaterials: The Monte Carlo Method",* International school on Nanostructure materials and membranes modeling and simulation, FORTH-ICE/HT, Patras, June 18-27, **2008**.
19. *"Atomistic Monte Carlo methodology for generating realistic flows of polymers guided by principles of non-equilibrium thermodynamics",* Polymer Physics Gordon Conference, Salve Regina University, Rhode Island, USA, June 29 - July 4, **2008.**
20. *"Hierarchical modeling of polymers at equilibrium and beyond-equilibrium conditions with emphasis on their mechanics and viscoelasticity",* DSM-Sabic R&D, The Netherlands, September 26, **2008**.
21. "*Hierarchical modeling of polymers at equilibrium and beyond equilibrium conditions with emphasis on viscoelasticity*", International seminar on Multi-scale modeling and simulation, Trondheim, Norway, October 13-14, **2008**.
22. "*Multiscale simulation of polymer melt viscoelasticity guided from non-equilibrium statistical thermodynamics: Atomistic Non-Equilibrium Molecular Dynamics coupled with Monte Carlo in an expanded statistical ensemble*", 6th International Discussion Meeting on Relaxations in Complex Systems, Rome, Italy, August 30 - September 5, **2009**.
23. "*Quantifying chain reptation in entangled polymer melts: Topological and dynamical mapping of atomistic simulation results onto the tube model*", Theory and Computer Simulation of Polymers", Moscow, Russia, May 31 - June 6, **2010**.
24. *"Modeling polymer melt viscoelasticity: Quantifying chain reptation in entangled polymer melts through a novel topological and dynamical mapping of atomistic simulation results onto the tube model*", International Workshop on Novel Simulation methods in Soft matter Systems (NSASM-2010)", Dresden, Germany, September 20-24, **2010**.
25. *"Atomic and electronic structure of polymer organic semiconductors: What we can learn from computer simulations at different scales*", 9th Hellenic Polymer Society Symposium (ELEP 2012), Thessaloniki, Greece, November 29-December 01, **2012**.
26. *"Interfacing molecular simulations with theories of polymer dynamics: the case of entangled polymer melts and polymer rings",* Department of Materials Science, University of Crete, Heraklion, Crete, March 01, **2013**.
27. *"Topological interactions in ring poly(ethylene oxide) melts and their correlation with conformational and rheological properties: A computer simulation study",* Ring Polymers: Advances and Applications, Heraklion, Crete, July 12-15, **2015**.
28. *Simulation of polymer melts beyond equilibrium using a non-dynamic method (GENERIC Monte Carlo) in an expanded ensemble*, Technical University of Eindhoven, Department of Mechanical Engineering, April 19, **2016.**
29. *Using nonequilibrium thermodynamics to extend atomistic Monte Carlo simulations of polymers beyond equilibrium*, Multiscale Simulation Methods for Soft Matter Systems, Darmstadt, Germany, October 4-6, **2016**.
30. *Atomistic Monte Carlo simulation of self-assembly in soft matter systems*, SCIMEETING Europe, Materials Modellig and Simulations Conference, Athens, Greece, June 21-23, **2017**.
31. *Fundamentals of Molecular Simulations*, Advances in the Mechanics and Chemistry of Adshesion: Training School in the course of the European Marie-Curie Training Project BioSmartTrainee, Paris, France, September 13-15, **2017**.
32. *Microscopic dynamics and threadings in ring polymers: A detailed computer simulation study*, Ring Polymers: Focused Workshop, Heraklion, Crete, September 25-27, **2017**.
33. *Molecular modelling of materials: making a difference in industry*, Plastics Update, 2nd edition,

Fribourg, Switzerland, November 9, **2017**.

34. *Topological constraimts in ring polymers*, 12th Hellenic Polymer Society Symposium (ELEP 2018), Ioannina, Greece, September 30 – October 03, **2018**.

TEACHING

Undergraduate Courses

1. "*Introduction to informatics I*", Laboratory, Department of Materials Science, University of Patras, Fall **2000** (with Dr. A. Terzis, Dr. E. Serpi, Dr. A. Vanakaras).
2. "*Introduction to informatics II*", Department of Materials Science, University of Patras, Spring **2002** (with Dr. A. Vanakaras, and Dr. M. Paspalakis).
3. "*Physical Chemistry II*", Department of Chemical Engineering, University of Patras, Spring **2003**, Spring **2004**, Spring **2005**, Spring **2006**, Spring **2007,** Spring **2009**, Spring **2010**, Spring **2011,** Spring **2013**.
4. "*Physical Chemistry*", Department of Chemical Engineering, University of Patras, Fall **2017** (with Prof. D. Kondarides), Fall **2018** (with Prof. D. Kondarides).
5. "*Special Topics of Physical Chemistry*", Department of Chemical Engineering, University of Patras, Fall **2003**, Fall **2004**, Fall **2005**.
6. *"Polymer rheology"*, Department of Chemical Engineering, University of Patras, Fall **2006**, Fall **2007**, Fall **2008,** Fall **2009**, Fall **2010**, Fall **2011**, Fall **2012**.

Graduate Courses

1. "*Computer simulation of polymers*", Interdepartmental Programme of Graduate Studies on "Polymer Science and Technology", University of Patras, Spring **1999,** Spring **2000,** Spring **2002** (with Dr. A. Terzis and Prof. D. Theodorou).
2. *Molecular Simulation and Statistical Mechanics*, Department of Chemical Engineering, University of Patras, Spring **2003**, Spring **2005**, Spring **2007**, Spring **2009**, Spring **2011**, Spring **2012**, Spring **2018**.
3. "*Polymer rheology and processing*", Interdepartmental Programme of Graduate Studies on "Polymer Science and Technology", University of Patras, Fall **2000**, Spring **2002** (with Prof. J. Tsamopoulos).
4. "*Graduate Thermodynamics*", Department of Chemical Engineering, University of Patras, Fall **2003**, Fall **2004**, Fall **2005**, Fall **2006**, Fall **2007,** Fall **2008,** Fall **2009**, Fall **2010**, Fall **2011**.
5. "*Polymer rheology*", Inter-departmental Programme of Graduate Studies in "Polymer Science and Technology", University of Patras, Fall **2003**, Fall **2004**, Fall **2005**, Fall **2006**, Fall **2007,** Fall **2008,** Fall **2009**, Fall **2010**, Fall **2011**, Fall **2012,** Fall **2017** (with Dr. D.G. Tsalikis).
6. *"Polymer rheology"*, Department of Chemical Engineering & Inter-Department Programe of Graduate Studies in "Polymer Science and Technology", University of Patras, Fall **2018** (with Dr. D.G. Tsalikis).
7. "*Advanced Course on: Molecular simulation of Complex Chemical Systems with Emphasis to Practical Applications*", Danish Technical University (DTU), Lyngby, Denmark, June 28-July 9, **2010**.
8. *"Theory of Open Quantum Systems",* A crash course based on the book by Breuer-Petruccione: "The Theory of Open Quantum Systems (Clarendon, Oxford University Press, 2002)", Department of Materials Science, ETH-Z, Switzerland, June 25-July 20, **2012**.

TEACHING AT ETH-Z

1. *Introduction to Nanomaterials Engineering (INE)",* Department of Mechanical Engineering, ETH-Z, **Fall 2016** (with Prof. S.E. Pratsinis and Dr. K. Wegner).
2. *Introduction to Nanomaterials Engineering (INE)",* Department of Mechanical Engineering, ETH-Z, **Fall 2017** (with Dr. R. Büchel).

STUDENT ADVISEMENT AS RESEARCHER AT FORTH-ICE/HT

Diploma Thesis students

1. John Hatzinikolaou (academic advisor: Prof. D. Theodorou, graduated in 1999)
2. Michalis Apostolakis (academic advisor: Prof. D. Theodorou, graduated in 1999)

3. Dimitris Prentzas (academic advisor: Prof. C. Galiotis, graduated in 1999)
4. Costas Doulas (academic advisor: Prof. D. Theodorou, graduated in 2002)
5. Aggeliki Yianoussaki (academic advisor: Prof. D. Theodorou, graduated in 2002)

Masters' Degree students
1. Dimitra Aggelopoulou (academic advisor: Prof. D. Theodorou, graduated in 2000)
2. Michalis Apostolakis (academic advisor: Prof. D. Theodorou, graduated in 2000)
3. Ioanna-Elisavet Mavrantza (academic advisor: Prof. C. Galiotis, graduated in 2000)
4. Georgia Schismenou (academic advisor: Prof. D. Theodorou, graduated in 2001)
5. Georgia Tsolou (academic advisor: Prof. D. Theodorou, graduated in 2001)

Ph.D. students
1. Evangelia Zervopoulou (academic advisor: Prof. D. Theodorou, graduated in 2000)
2. Vagelis Harmandaris (academic advisor: Prof. D. Theodorou, graduated in 2001)
3. Nikos Karayiannis (academic advisor: Prof. D. Theodorou, graduated in 2002)
4. Kostas Daoulas (academic advisor: Prof. D. Photinos, graduated in 2003)

STUDENTS ADVISEMENT, DEPARTMENT OF CHEMICAL ENGINEERING, UNIVERSITY OF PATRAS

Diploma Thesis students
1. Pavlos Stephanou (graduated in 2006)
2. Eva Lionta (graduated in 2010)
3. Vasilis Georgilas (graduated in 2010)
4. Eirini Goudeli (graduated in 2012)
5. Katiana Efstratiou (graduated in 2013)
6. Aggeliki Chatzintouna (graduated in 2013)
7. Apostolos Ziovas (graduated in 2014)
8. Ioanna Mavrikou (graduated in 2014)
9. Andreas Doukas (graduated in 2014)
10. George Papadopoulos (graduated in 2014)
11. Christos Tsakonas (graduated in 2014)
12. Lina Aggelaki (graduated in 2015)
13. Artemis Charalampidou (graduated in 2015)
14. Maria Koukouta (graduated in 2015)
15. Spyros Agorgiannitis (graduated in 2016)
16. Dimitris Mallios (graduated in 2016)
17. Ioanna Tsimouri (graduated in 2016)
18. Eleni Xygki (graduated in 2017)
19. Costantinos Kasidiaris (2012-today)
20. Christos Georgantopoulos (2016- to date)
21. Eleni Chousa (2016- to date)
22. Constantinos Papadopoulos (2016- to date)
23. Georgios Zygouris (2016- to date)
24. Alexandros Tsamopoulos (2016- to date)
25. Despoina Rigou (2017- to date)
26. Evaggelia Kriti (2017- to date)
27. Anna Katsarou (2017- to date)

Masters' Degree students
1. Antigoni Theodoratou (graduated in 2010)
2. Nikos Stratikis (graduated in 2011)
3. Thanasis Koukoulas (graduated in 2012)
4. Elena Karahaliou (graduated in 2012)
5. Flora Tsourtou (graduated in 2013)
6. Emmanouil Skountzos (graduated in 2013)

7. Panagiotis Alatas (graduated in 2013)
8. Takis Mermigkis (graduated in 2014)
9. George Papadopoulos (2014- to date)
10. Ioanna Tsimouri (graduated in 2018)
11. Dimitris Malios (2016-2017)

Ph.D. students
1. Katerina Foteinopoulou (co-advisement with Prof. J. Tsamopoulos and C. Toprakcioglou, graduated in 2005)
2. Georgia Tsolou (graduate in 2005)
3. Orestis Alexiadis (graduated in 2007)
4. Pavlos Stephanou (graduated in 2011)
5. Alexandros Anastassiou (graduated in 2013)
6. Thanasis Koukoulas (2012- to date)
7. Elena Karahaliou (2012- to date)
8. Emmanouil Skountzos (2013- to date)
9. Panagiotis Alatas (2013- to date)
10. Flora Tsourtou (2014- to date)
11. Takis Mermigkis (2015- to date)
12. Dimitris Mintis (2016- to date)

Post-Doctoral Collaborators
1. Nikos Karayiannis (2002-2006)
2. Vagelis Harmandaris (2003-2005)
3. Kostas Daoulas (2003-2005)
4. Katerina Foteinopoulou (2005-2006)
5. Georgia Tsolou (2005-2011)
6. Chunggi Baig (2006-2012)
7. Orestis Alexiadis (2009-2014)
8. Dimitris Tsalikis (2011- to date)
9. Katerina Karadima (2013- to date)
10. Stavros Peroukidis (2017- to date)
11. Chara Alexiou (2017-to date)

STUDENT ADVISEMENT, ETH-ZURICH, PARTICLE TECHNOLOGY LABORATORY, DEPARTMENT OF MECHANICAL AND PROCESS ENGINEERING

Diploma Thesis students
1. Saskia Kohler (academic advisor: Prof. S.E. Pratsinis, graduated in 2015)
2. Natalia Smatsi (academic advisor: Prof. S.E. Pratsinis, graduated in 2018)

Masters' Degree students
1. Vasil Vasilev (academic advisor: Prof. S.E. Pratsinis, graduated in 2017)
2. Natalia Smatsi (academic advisor: Prof. S.E. Pratsinis, Sept. 2017-to date)

Ph.D. students
1. Anastasia Spyrogianni (academic advisor: Prof. S.E. Pratsinis, graduated in 2017)
2. Alexander Weyman (academic advisor: Prof. H.C. Öttinger, 2017-to date)

Post-Doctoral Collaborators
1. Nikolaos Lempesis (2017-today)

REVIEWER FOR SCIENTIFIC JOURNALS

Reviewer for manuscripts submitted for consideration for publication in:
- *ACS Applied Nano Materials*
- *ACS Macro Letters*

- *ACS Nano Letters*
- *Advanced Composite Letters*
- *AICHE Journal*
- *Cellulose*
- *Chemical Engineering Research and Design*
- *Chemical Engineering Science*
- *Computational Materials Science*
- *Computers & Chemical Engineers*
- *Computer Physics Communications*
- *European Polymer Journal*
- *Europhysics Letters*
- *Industrial & Engineering Chemistry Research*
- *Journal of Advanced Physics*
- *Journal of the American Chemical Society*
- *Journal of Applied Physics*
- *Journal of Chemical Physics*
- *Journal of Crystal Growth*
- *Journal of Fluid Mechanics*
- *Journal of Fluorine Chemistry*
- *Journal of Hazardous Materials*
- *Journal of Materials Chemistry C*
- *Journal of Membrane Science*
- *Journal of Molecular Modeling*
- *Journal of Nanostructured Polymers and Nanocomposites*
- *Journal of Non-Equilibrium Thermodynamics*
- *Journal of Non-Newtonian Fluid Mechanics*
- *Journal of Polymer Science, Part B: Polymer Physics*
- *Journal of Physical Chemistry A,B,C*
- *Journal of Rheology*
- *Journal of Supercritical Fluids*
- *Korea-Australia Rheology Journal*
- *Fluid Phase Equilibria*
- *Langmuir*
- *Macromolecules*
- *Macromolecular Rapid Communications*
- *Macromolecular Theory and Simulation*
- *Materials Chemistry and Physics*
- *Molecular Simulation*
- *Nano Letters*
- *New Journal of Physics*
- *Physica A*
- *Physical Chemistry Chemical Physics (PCCP)*
- *Physics Letters A*
- *Physical Review E*
- *Physical Review Fluids*
- *Physical Review Letters*
- *Physics of Fluids*
- *Polymer*
- *Reactive and Functional Polymers*
- *Rheologica Acta*
- *Royal Society Advances*
- *Scientific Reports*
- *Soft Matter*
- *Theoretical and Computational Polymer Science*

REVIEWER FOR FUNDING ORGANIZATIONS

Reviewer for proposals submitted for consideration for funding in:

- *Dutch Polymer Institute (DPI, The Netherlands)*
- *National Science Foundation (NSF, USA)*
- *The Petroleum Research Fund (ACS-PRF, USA)*
- *Greek Secretariat For Research and Technology (GSRT, Greece)*
- *Greek Ministry of Education and Religious Affairs (Greece)*
- *Research Committee, National Technical University of Athens (NTUA, Greece)*

ORGANIZATION OF SCIENTIFIC MEETINGS

1. Member, Organizing Committee, *2nd International Meeting of the Hellenic Society of Rheology*, Heraklion, Crete, Greece, August 31-September 1st, **1998**.
2. Chairman, Organizing Committee, *3rd International Meeting of the Hellenic Society of Rheology*, Patras, Greece, June 10-June 14, **2001** (Conference dedicated to Prof. Andreas Acrivos on the occasion of his retirement from the Levich Institute, The City College of the City University of New York).
3. Member, Scientific Committee, *5th Panhellenic Conference on Polymers*, Heraklion, Crete, Greece, December 15-17, **2001**.
4. Member, Organizing Committee, *4th Panhellenic Chemical Engineers' Conference*, Patras, Greece, May 30-June 1, **2003**.
5. Member, Scientific Committee, *2nd International Workshop and Summer School of Nonequilibrium Thermodynamics and Complex Fluids*, Princeton, USA, August 14-17, **2003**.
6. Member, Organizing Committee, *3rd Annual European Rheology Conference (AERC-2006)*, Crete, Greece, April 27-29 **2005.**
7. Chairman, Organizing and Scientific Committee, *4th International Workshop on Non-equilibrium Thermodynamics and Complex Fluids (IWNET)*, Rhodes, Greece, September 4-7, **2006**.
8. Member, Organizing Committee, *11th International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD 2007)*, Crete, Greece, May 20-25, **2007**.
9. Vice-Chair, Organizing and Scientific Committee, *15th International Workshop of Numerical Methods for Non-Newtonian Flows*, Rhodes, Greece, June 14-17, **2007**.
10. Member, Scientific Committee, *4th International Conference from Scientific Computing to Computational Engineering (4th IC-SCCE)*, Athens, Greece, July 7-10, **2010**.
11. Member, Organizing and Scientific Committee, *7th International Workshop on Non-equilibrium Thermodynamics and Complex Fluids (IWNET 2015)*, Hilvarenbeek, The Netherlands, July 6-10, **2015**.

SERVICES TO THE DEPARTMENT OF CHEMICAL ENGINEERING

1. Seminars Committee
   - Chairman: 2003-2005, 2005-2007
   - Member: 2007-2009, 2009-2011, 2011-2013
2. Committee of Undergraduate Studies, Member, 2003-2005
   - Member: 2003-2005, 2005-2007, 2007-2009, 2009-2011,2011-2014
3. Committee of Graduate Studies, Chairman, 2007-2009
   - Member: 2005-2007
   - Chairman: 2007-2009, 2009-2011, 2011-2014
   - Co-chairman: 2017-today
4. Committee of Research and Academic Development, Member, 2007-2009
   - Member: 2005-2007, 2007-2009
5. Committee of Computing and Network Infrastructure
   - Member: 2009-2011, 2011-2014
6. Department's Internal Evaluation Committee
   - Member: 2011-2014

REFERENCES

Prof. Antony N. Beris Prof. Doros Theodorou

Department of Chemical Engineering
University of Delaware
Newark, DE 19716
USA
e-mail: beris@udel.edu
tel.: +1 302 831 4416

Prof. John Tsamopoulos
1 Caratheodori Street
Department of Chemical Engineering
University of Patras
Patras GR 26500, Greece
e-mail: tsamo@chemeng.upatras.gr
tel.: +30 2610 997 203

Prof. Dimitris Vlassopoulos
Department of Materials Science
& FORTH-IESL
P.O. Box 2208
710 03 Heraklion Crete, Greece
e-mail: dvlasso@iesl.forth.gr
tel.: +30 2810 391 469

Prof. Hans-Christian Öttinger
Department of Materials
Institute of Polymers
ETH, CNB E 92
CH-8092 Zürich, Switzerland
e-mail: hco@mat.ethz.ch
tel.: +41 1 632 3127

Prof. Greg Rutledge
Department of Chemical Engineering
Room 66-368
77 Massachusetts Avenue
Cambridge, MA 02139, USA
e-mail: rutledge@mit.edu
tel.: +617 253 0171

Prof. Roland Keunings
Division of Applied Mechanics
Université Catholique de Louvain
Av. Georges Lemaître
B-1348 Louvain-la-Neuve
Belgium
e-mail: rk@mema.ucl.ac.be
tel.: +32 104 72350

Prof. Sotiris E. Pratsinis
ETH Zurich
Institut f. Verfahrenstechnik
Zurich 8092
Switzerland
E-Mail: sotiris.pratsinis@ptl.mavt.ethz.ch

National Technical University of Athens
Department of Chemical Engineering
9 Heroon Polytechniou St., Zographou
Athens, Greece GR-157 80
e-mail: doros@chemeng.ntua.gr
tel.: +30 210 772 3157

Prof. Ioannis G. Economou
Professor, Chemical Engineering Program
Texas A&M University at Qatar
336B Texas A&M Engineer. Build., Education City
PO Box 23874, Doha, Qatar
e-mail: ioannis.economou@qatar.tamu.edu
tel.: + 974 4423 0549, + 974 3391 6158

Prof. George Fytas
Department of Materials Science
& FORTH-IESL
P.O. Box 2208
710 03 Heraklion Crete, Greece
e-mail: fytas@iesl.forth.gr
tel.: +30 2810 391 469

Prof. Manolo Laso
ETSII
Department of Chemical Engineering
Jose Gutierrez Abascal 2
28006 Madrid, Spain
e-mail: laso@diquima.upm.es
tel.: +34 91 3363015

Prof. Efthimios Kaxiras
Lyman Laboratory 333
Department of Physics
Harvard University
Cambridge MA 02138
e-mail: kaxiras@kriti.harvard.edu
tel.: +1 617 495 7977

Dr. Rudy Koopmans
R&D External Technologies Europe
Dow Benelux N.V.
P.O. Box 48
4530 AA Terneuzen
The Netherlands
e-mail: rjkoopmans@dow.com
tel.: +31 115 673680

Phone: +41 44 632 31 80