VLASIS G. MAVRANTZAS

OFFICE ADDRESS 1
University of Patras
Departmnet of Chemical Engineering
1 Caratheodori Street
Patras, GR 26500
Greece
e-mail: vlasis@chemeng.upatras.gr
tel.: +30 6944 60 25 80

HOME ADDRESS 1
13A Iasonos Street
Xylokastro
Korinthia, GR 20400
Greece

OFFICE ADDRESS 2
ETH Zürich
Department of Mechanical and Process Engineering
ML F 14.2
Sonneggstrasse 3, 8092 Zürich
Switzerland
e-mail: vlasiosm@mat.ethz.ch
tel.: + 41 44 632 8503, +41 78 735 2088

HOME ADDRESS 2
Lerchenberg 6
8046 Zürich
Switzerland

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
- Polymer Dynamics and Rheology
- Finite-Element and Spectral-Element Numerical Methods

RESEARCH INTERESTS

- Modeling and simulation of polymers and of soft nanostructured materials at multiple time and length scales (atomistic, mesoscopic, macroscopic)
- Thermodynamics of complex fluids under non-equilibrium conditions and constitutive modeling of polymer viscoelasticity
- Molecular Simulation of the phase state and physicochemical properties of atmospheric organic aerosol particles
- Hydrogels and their physicochemical properties
- Relativistic Hydrodynamics from Non-Equilibrium Thermodynamics
- 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

Lecturer (September 2016- today)
Department of Mechanical and Process Engineering, ETH Zürich, Switzerland (initially with Prof. Sotiris Pratsinis, now with Prof. Mark Tibbitt)

Guest Professor (September 2014- September 2016)
Department of Mechanical and Process Engineering (with Prof. Sotiris 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 (FORTH-ICE/HT) & Department of Chemical Engineering, University of Patras, Patras, Greece

Military Service (May 1994-December 1995)
War Material Corps, Didymoteicho, Evros & 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)

DISTINCTIONS

- Section Editor-in-Chief, Polymer Physics, *Polymers*, MDPI (since 2020)
- On the Editorial Board, *J. of Non-Equilibrium Thermodynamics* (to join in 2027)
- Associate Editor, Soft Matter Physics, *Frontiers in Physics* (since 2018)
- Member, International Advisory Board, *Macromolecular Theory and Simulation*, Wiley-VCH, Germany (since 2005).

JOURNAL COVERS

1. Front Cover for the article: "*Structure and conformation of a crystalline P3HT film adsorbed on an alkanethiol self-assembled monolayer deposited on gold*", by E.N. Skountzos, F. von Wrochem, and **V.G. Mavrantzas**,* *Macromol. Theory & Simul.* **2020**, 2000010.
2. Inside Back Cover Page for the article: "*3-Arm Star Pyrene-Functional PMMAs for efficient exfoliation of Graphite in Chloroform: Fabrication of Graphene-Reinforced Fibrous Veils*", by S.S. Gkermpoura, K.D. Papadimitriou, E.N. Skountzos, I. Polyzos, M.G.P. Carbone, A. Kotrotsos, **V.G. Mavrantzas**, C. Galiotis, and C. Tsitsilianis,* *Nanoscale* **2019**, 11, 915-931.
3. Front Cover for the article: "*Molecular simulation of the high temperature phase behaviour of α-unsubstituted sexithiophene*", by F.D. Tsourtou, E.N. Skountzos, S.D. Peroukidis, and **V.G. Mavrantzas**,* *Soft Matter* **2018**, 14, 8253 – 8266.
4. Front Cover Page for the article: "*Molecular modelling combined with advanced chemistry for the rational design of efficient graphene dispersing agents*", by K.D. Papadimitriou, E.N. Skountzos, S.S. Gkermpoura, I. Polyzos, **V.G. Mavrantzas**, C. Galiotis, and C. Tsitsilianis,* *ACS Macro Lett.* **2016**, 5, 24−29.
5. Front Cover Page for the article: "*Determination of the mechanical properties of a poly(methyl methacrylate) nanocomposite with functionalized graphene sheets through detailed atomistic simulations*", by E.N. Skountzos, A. Anastassiou, **V.G. Mavrantzas**,* and D.N. Theodorou, *Macromolecules* **2014**, 47, 8072–8088.

BEST POSTER AWARDS

1. Best Poster Award for the paper: "Glass transition temperature of organic compounds making up atmospheric nanoparticles from molecular dynamics simulations", by P. Siachouli, K.S. Karadima, V.G. Mavrantzas, and S.N. Pandis, *13th Panhellenic Chemical Engineers Conference*, Patras, Greece, June 2-4, **2022**.
2. Best Poster Award for the paper: "Conformational and dynamic properties of DNA minicircles in aqueous solution from atomistic molecular dynamics simulations", by T.S. Alexiou, D.G. Tsalikis, P.V. Alatas and V.G. Mavrantzas, *12th Hellenic Polymer Society International Conferemce (ELEP 2018)*, Ioannina, Greece, September 30-October 3, **2018**.
3. Best Particle Technology Forum (PTF) Student Poster Award for the paper: "Settling rate of agglomerates consisting of polydisperse primary particles by Brownian Dynamics", by A. Spyrogianni, K.S. Karadima, E. Goudeli, V.G. Mavrantzas, and S.E. Pratsinis, *AIChE Annual Meeting*, Minneapolis, USA, October 29 - November 03, **2017**.
4. Best Poster Award for the paper: "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", by P. V. Alatas, D. G. Tsalikis, and V.G. Mavrantzas, *11th Hellenic Polymer Society Conference (ELEP 2016)*, Heraklion, Crete, Greece, November 3-5, **2016**.
5. Best Poster Award for the paper: "Microscopic dynamics and topology of polymer rings immersed in a host matrix of longer linear polymers: Results from a detailed molecular

dynamics study and comparison with experimental data", by D. G. Tsalikis, and V.G. Mavrantzas, *2nd Workshop of Graduates and Post-Doncs in Chemical Engineering Sciences*, Patras, Greece, September 21, **2016**.

BEST ORAL PRESENTATION AWARDS

1. Best Oral Presentation Award for the paper: "Study of the structure and mechanism of antimicrobial action of short peptides derived from keratin (KAMPs) using molecular dynamics simulations", by P. Apostolaki, K.S. Karadima, and V.G. Mavrantzas, *13th Panhellenic Chemical Engineers Conference*, Patras, Greece, June 2-4, **2022**.
2. Best Oral Presentation Award for the paper: "Detailed atomistic molecular dynamics study of the conformation and diffusion of small circular and linear DNA molecules in dilute solution", by T.S. Alexiou, D.G. Tsalikis, P.V. Alatas, and V.G. Mavrantzas, *5th Workshop of Graduates and Post-Docs in Chemical Engineering Sciences*, Patras, Greece, November 6, **2019**.
3. Best Oral Presentation Award for the paper: "Atomistic simulations combined with advanced modelling for the prediction of the microscopic dynamics of polymer nanocomposites", by E.N. Skountzos, D.G. Tsalikis, P.S. Stephanou, and V.G. Mavrantzas, *5th Workshop of Graduates and Post-Docs in Chemical Engineering Sciences*, Patras, Greece, November 06, **2019**.
4. Best Oral Presentation Award for the paper: "Atomistic simulation of DNA minicircles in aqueous solution", by T.S. Alexiou, D.G. Tsalikis, P.V. Alatas, and V.G. Mavrantzas, *4th Workshop of Graduates and Post-Docs in Chemical Engineering Sciences*, Patras, Greece, October 3, **2018**.

PRIZES AND AWARDS

- 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, USA, 1993-1994
- Competitive Fellowship, University of Delaware, USA, 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)

ADMINISTRATIVE POSITIONS

- Secretary-Treasurer, Hellenic Society of Rheology (HSR), Sept. 2006-Sept. 2023
- President, Hellenic Society of Rheology (HSR), Sept. 2004-Sept. 2006
- Director, Inter-department Programme of Graduate Studies on "Polymer Science and Technology", University of Patras, 2003-2013

PARTICIPATION IN RESEARCH AND DEVELOPMENT PROJECTS

NATIONAL PROJECTS

PROSMAK [1]:

- 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 national contribution: 220 kEuro
- Contribution to the Lab: 50 kEuro
- Duration: 2002-2005
- Project Coordinator: V.G. Mavrantzas

ESOPO [2]

- 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 national contribution: 193.7 kEuro
- Contribution to the Lab: 46 kEuro
- Duration: 2002-2005
- Project Coordinator: V. Gregoriou

AKMON 2004 [3]

- 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 [4]

- 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 [5]

- 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 national contribution: 50 kEuro
- Contribution to the Lab: 25 kEuro
- Duration: 2005-2007
- Project coordinator: J. Tsamopoulos

HERACLITUS [6]

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

MEKKA [7]

- 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
- Contribution to the Lab: 80 kEuro
- Duration: 2011-2013
- Project coordinator: V.G. Mavrantzas

THALES [8]

- 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 [9]

- 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

RINGS [10]

- National research project (GSRT, Support of reserachers with emphasis to new researchers) titled: *Conformational and transport properties of solutions of synthetic and biological cyclic polymers: theory and atomistic simulation (RING-Solutions)*
- Contract No: 5004866
- Partners: FORTH-ICE/HT
- Total national contribution: 59,85 kEuro
- Contribution to the Lab in Patras: 59.85 kEuro
- Duration: 2018-2019
- Project coordinator: V.G. Mavrantzas

PNC_RHEO [11]

- National research project (GSRT, Support of researchers with emphasis to young researchers) titled: *Study of the rheology of polymer nanocomposite melts by combining molecular simulations and rheological constitutive modelling (PNC_Rheo)*
- Partners: UPatras
- Total national contribution: 41.5 kEuro
- Contribution to the Lab in Patras: 41.5 kEuro
- Duration: 2019-2020
- Project coordinator: V.G. Mavrantzas

RINGS [12]

- National research project (FORTH Synergy Grant) titled: *Shear and extensional rheology of entangled ring polymer melts (RINGS)*
- Partners: FORTH-IESL, FORTH-ICE/HT

- Total national contribution: 80 kEuro
- Contribution to the Lab in Patras: 25 kEuro
- Duration: 2019-2021
- Project coordinator: D. Vlassopoulos

HEFRI [13]

- National research project (HFRI, Basic Research Financing Action) titled: *Thermal stimuli-responsive 3D printed electroactive polymer nanocomposites towards 4D "programmable" geometries (THUNDER)*
- Partners: HMU, FORTH, UPatras, AUTH
- Total national contribution: 339.5 kEuro
- Contribution to the Lab in Patras: 41.8 kEuro
- Duration: 2024-2026
- Project coordinator: L. Tzounis (HMU)
- Project leader from UPatras: V.G. Mavrantzas

HEFRI [13]

- National research project (easyHPC@eco.plastics.industry) titled: *Ανάπτυξη Δικτύου των Ευρωπαϊκών Κόμβων Ψηφιακής Καινοτομίας – ΕΚΨΚ (European Digital Innovation HUBs – EDIHs) που έχουν λάβει Σφραγίδα Αριστείας από το Πρόγραμμα «Ψηφιακή Ευρώπη»*
- Partners: UPatras
- Total budget: 3,000 kEuro
- Contribution to the Lab in Patras: 300 kEuro
- Duration: 2024-2027
- Project coordinator: Y. Dimakopoulos (UPatras)
- Project leader from LSTM: V.G. Mavrantzas

<u>EUROPEAN (EC) PROJECTS</u>

GeMColloidS [1]

- 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

PMILS [2]

- 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

MODIFY [3]

- 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

PEPPER [4]

- 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 [5]

- 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 [6]

- 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

BioSmartTrainee [7]

- 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

FORCE [8]

- 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

RELIANCE [9]

- EC research project (HORIZON-CL4-2021-RESILIENCE-01) titled: *Smart Response self-desinfected biobased nanocoated surfaces for healthier environments (RELIANCE)*
- Contract No: RELIANCE
- Partners: Fundación Tekniker, Maier S. Coop., Maier Technology Centre S. Coop., Millidyne, Polyrise, Centexbel, UPatras, Institut National de l'Environment et des Risques, Universita degli studi di Roma Tor Vergata, Policlinico Militare di Roma, HESSO, Europroject OOD, Molecular Plasma Group, ARCELIK A.S., Alsico High Tech
- Total EC contribution: 5,757 kEuro
- EC contribution to the Lab in Patras: 294.1 kEuro
- Duration: 2022-2026
- Project coordinator: E. Aranzabe (Fundación Tekniker, ES)
- Project leader from UPatras: V.G. Mavrantzas

<u>INDUSTRIAL PROJECTS</u>

DOW Chemicals Industrial Project I [1]

- 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

DOW Chemicals Industrial project II [2]

- 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

Limmat [3]

- Limmat Foundation donation project (MuSiComPS) titled: *Multiscale Simulations of Complex Polymer Systems (MuSiComPS)*
- Contract No: MuSiComPS
- Partners: NTUA, UPatras
- Total Limmat Foundation contribution: ~1000 kEuro
- Contribution to the Lab: 320 kEuro
- Duration: 2015-2020
- Project coordinator: D.N. Theodorou
- Project leaders from UPatras: V.G. Mavrantzas, J. Tsamopoulos

Micelles [4]

- Industrial research project with Unilever (UK) titled: *Simulation of Isotropic Liquids*
- Contract No: Research contract with Unilever (UK)
- Partners: UPatras (coordinator), Unilever (UK)
- Total budget: 245 kEuro
- Contribution to the Lab: 295 kEuro
- Duration: 2021-2023
- Project leader from UPatras: V.G. Mavrantzas

OTHER 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

NATO CRG 2001 [2]

- 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

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).
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70. P.S. Stephanou, D.G. Tsalikis, E.N. Skountzos, **V.G. Mavrantzas**, "Modelling of polymer nanocomposite melts based on principles of nonequilibrium thermodynamics and the findings of detailed nonequilibrium molecular dynamics simulations", *11th Panhellenic Chemical Engineers Conference*, Salonica, Greece, May 25-27, **2017.**

71. 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.**
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81. P.V. Alatas, **V.G. Mavrantzas**, H.C. Öttinger, "Analytical calculation of the propagator of the dissipative quantum φ^4 theory up to 3rd order from nonequilibrium thermodynamics", *13th Panhellenic Chemical Engineers Conference*, Patras, Greece, June 2-4, **2022**.
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85. D.G. Tsalikis, P.G. Mermigkis, Ch. Christopoulou, I. Stott, **V.G. Mavrantzas**, "Salt concentration effects on the morphology of micellar solutions of ionic surfactants and their mixtures with zwitteronic co-surfactants", *13th Panhellenic Chemical Engineers Conference*, Patras, Greece, June 2-4, **2022**.
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PRESENTATIONS (speaker underlined)

1. **V.G. Mavrantzas**, A.N. Beris, "Theoretical study of the effects of solid/fluid interface on the rheology of polymer solutions", *March Meeting of the American Physical Society*, Cincinnati, March 18-22, **1991**.
2. **V.G. Mavrantzas**, A.N. Beris, "Theoretical study of the effects of solid/fluid interface on the rheology of polymer solutions", *"Symposium on Interfacial Phenomena in Viscoelastic Flows*" organized by the Fluid Mechanics Committee of the Applied Mechanics Division of ASME, Columbus, June 16-19, **1991**.
3. **V.G. Mavrantzas**, A.N. Beris, "Theoretical Study of wall effects on the rheology of dilute polymer solutions", *Society of Rheology Meeting*, Rochester, October 20-24, **1991**.
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**.
7. **V.G. Mavrantzas**, A.N. Beris, "Stress-induced polymer migration phenomena in simple viscometric flows", *Society of Rheology Meeting*, Boston, October 17-21, **1993**.
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10. **V.G. Mavrantzas**, D.N. Theodorou, "From chain chemical structure to polymer melt elasticity: The implementation of new Monte Carlo techniques'', *EPF Annual Meeting*, Aghia Pelaghia, Crete, Greece, October 7-11, **1996**.
11. **V.G. Mavrantzas**, D.N. Theodorou, "From chain chemical structure to polymer melt elasticity: The implementation of new Monte Carlo techniques", *1st Panhellenic Chemical Engineers' Conference*, Patras, Greece, May 29-31, **1997**.
12. V.A. Harmandaris, **V.G. Mavrantzas**, D.N. Theodorou, "From chemical structure to polymer processing: Atomistic simulation of the viscoelasticity of linear polyethylene melts", *4th Hellenic Polymer Society Symposium (ELEP 1997)*, Patras, Greece, November 20-22, **1997**.
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14. E. Zervopoulou, **V.G. Mavrantzas**, D.N. Theodorou, "Atomistic simulation of the solubility of small alkanes in long polyethylene melts", *2nd Panhellenic Chemical Engineers' Conference*, Salonica, Greece, May 27-29, **1999**.
15. V.A. Harmandaris, **V.G. Mavrantzas**, D.N. Theodorou, "Atomistic simulation of the stress relaxation experiment after cessation of steady-state uniaxial elongation", *2nd Panhellenic Chemical Engineers' Conference*, Salonica, Greece, May 27-29, **1999**.
16. M. Apostolakis, J. Hatzinicolaou, **V.G. Mavrantzas**, "Stress-induced polymer migration effects in the Taylor-Couette device: Numerical calculations with spectral elements", *2nd Panhellenic Chemical Engineers' Conference*, Salonica, Greece, May 27-29, **1999**.
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properties of long-chain polyethylene melts from detailed atomistic simulations on uniaxially stretched melt configurations", *XIII International Congress on Rheology*, Cambridge, UK, August 20-25, **2000**.

21. **V.G. Mavrantzas**, A.N. Beris, "Polymer depletion phenomena near a solid surface: Modeling the effect of a shear flow", *XIII International Congress on Rheology*, Cambridge, UK, August 20-25, **2000.**
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23. M. Apostolakis, **V.G. Mavrantzas**, "Polymer diffusion in inhomogeneous flow fields: pseudospectral calculations in the Taylor-Couette geometry", *35th Annual Meeting of the French Society of Rheology*, Grenoble, October 23-25, **2000**.
24. N.Ch. Karayiannis, **V.G. Mavrantzas**, D.N. Theodorou, "Effects of Jump Rate Distribution and Spatial Heterogeneity", *AIChE Annual Meeting*, Los Angeles, November 13-17, **2000**.
25. V.A. Harmandaris, **V.G. Mavrantzas**, D.N. Theodorou, "Rheological Properties of Polymer Melts from Molecular Constitution", *AIChE Annual Meeting*, Los Angeles, November 13-17, **2000.**
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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**.
28. K. Daoulas, A.F. Terzis, **V.G. Mavrantzas**, "Melts of macromolecules grafted on a hard surface or graphite: Detailed atomistic simulation of their interfacial structure", *3rd Panhellenic Chemical Engineers' Conference*, Athens, Greece, May 31-June 02, **2001**.
29. V.A. Harmandaris, **V.G. Mavrantzas**, D.N. Theodorou, "Prediction of the viscoelastic properties of high-molecular weight polymer melts through molecular dynamics atomistic simulations", *3rd Panhellenic Chemical Engineers' Conference*, Athens, Greece, May 31-June 02, **2001**.
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33. K.Ch. Daoulas, A.F. Terzis, **V.G. Mavrantzas**, "Detailed end-bridging Monte Carlo simulations of grafted polyethylene melts", *Euroconference on Interfaces and Thin Films of Polymers and Colloidal Systems,* Acquafredda di Maratea, Italy, September 8-13, **2001**.
34. **V.G. Mavrantzas,** M. Apostolakis, A.N. Beris, "Stress-induced migration effects in the Taylor-Couette flow: Numerical simulation of the stress-concentration coupling", *73rd Annual Meeting of the Society of Rheology*, Bethesda, Maryland, USA, October 21-25, **2001.**
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36. Karayiannis, N.C.; **Mavrantzas, V.G.**; Theodorou, D.N., "A new method for the rapid equilibration of atomistic macromolecular model systems of a precisely defined chemical architecture", Proceedings*, 5th Hellenic Polymer Society Symposium (ELEP 2001)*, Heraklion, Crete, December 15-17, **2001**.
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38. K.Ch. Daoulas, **V.G. Mavrantzas**, V.A. Harmandaris, K. Foteinopoulou, D.N. Theodorou, "Atomistic Monte Carlo simulations and SCF Calculations of polymers at interfaces"*, 4th GRACM Congress on Computational Mechanics*, Patras, Greece, June 27-29, **2002**.

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46. G. Tsolou, **V.G. Mavrantzas**, D.N. Theodorou, "Atomistic molecular dynamics simulations of cis-1,4 polybutadiene melts", *4th Panhellenic Chemical Engineers' Conference*, Patras, Greece, May 29-31, **2003.**
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48. **V.G. Mavrantzas**, "Thermodynamically founded hierarchical methodologies for the simulation of polymer melts beyond equilibrium: Detailed atomistic simulation of polymer melt viscoelasticity", *3rd International Workshop on Non-Equilibrium Thermodynamics and Complex Fluids (3rd IWNET)*, Princeton, USA, August 14-17, **2003**.
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259. D.G. Mintis, **V.G. Mavrantzas**, "All atomistic molecular dynamics study of the effect of pH and molecular weight on structure and dynamics of the weak polyelectrolyte poly(acrylic acid)", *12th Panhellenic Chemical Engineers Conference*, Athens, May 29-31, **2019**.
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261. D.G. Mintis, D. Rigou, **V.G. Mavrantzas**, "Detailed molecular dynamics simulation study of the phase boundary for complex coacervation between poly(acrylic acid) and poly(N,N-dimethyl amino ethyl methacrylate) (poster presentation)", *12th Panhellenic Chemical Engineers Conference*, Athens, May 29-31, **2019**.
262. T. Alexiou, E. Kriti, D. Loukas, **V.G. Mavrantzas**, "Atomistic molecular dynamics simulation of the diffusive behavior of short linear DNA molecules in dilute aqueous solutions: Comparison with experiments and theoretical models (poster presentation)", *12th Panhellenic Chemical Engineers*

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264. T.S. Alexiou, D.G. Tsalikis, P.V. Alatas, **V.G. Mavrantzas**, "Conformational and transport properties of small circular DNA molecules in dilute solution: A detailed molecular dynamics simulation study", *Frontiers in Polymer Science 2019*, Budapest, Hungary, June 05-08, **2019**.
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270. P.S. Stephanou, I.Ch. Tsimouri, G.C. Georgiou, **V.G. Mavrantzas**, "Understanding the rheological behaviour of blood from a non-equilibrium thermodynamics perspective", *9th International Meeting of the Hellenic Society of Rheology (HSR 2019)*, Pythagorion, Samos, Greece, June 23-27, **2019**.
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272. F.D. Tsourtou, S.D. Peroukidis, **V.G. Mavrantzas**, "Novel mesomorphic behavior of alpha-unsubstituted oligothiophens: a Computer simulation study", *XXXIV Panhellenic Conference on Solid State Physics and Materials Science*, Patras, Greece, September 11-14, **2019**.
273. D.G. Tsalikis, **V.G. Mavrantzas**, D. Vlassopoulos, "RINGS: Shear and extensional rheology of entangled ring polymer melts", *12th FORTH Retreat Conference (FORTH 2019)*, Patras, Greece, October 15-16, **2019**.
274. K.S. Karadima, **V.G. Mavrantzas**, S.N. Pandis, "Molecular dynamics study of the morphology of ultrafine multicomponent organic aerosol", *12th FORTH Retreat Conference (FORTH 2019)*, Patras, Greece, October 15-16, **2019**.
275. T.S. Alexiou, D.G. Tsalikis, P.V. Alatas, **V.G. Mavrantzas**, "Detailed atomistic molecular dynamics study of the conformation and diffusion of small circular and linear DNA molecules in dilute solution", *12th FORTH Retreat Conference (FORTH 2019)*, Patras, Greece, October 15-16, **2019**.
276. P.G. Mermigkis, **V.G. Mavrantzas**, "Free and accessible volume of small penetrants in a poly(methyl methacrylate)-Carbon Nanotube nanocomposite via Monte Carlo integration", *12th FORTH Retreat Conference (FORTH 2019)*, Patras, Greece, October 15-16, **2019**.
277. D.G. Mintis, M. Dompé, M. Kamperman, **V.G. Mavrantzas**, "A combined experimental and Molecular Dynamics study to investigate the effect of polymer concentration on the structure and dynamics of short weak polyelectrolyte poly(N,N-dimethylaminoethyl methacrylate) in aqueous solution", *12th FORTH Retreat Conference (FORTH 2019)*, Patras, Greece, October 15-16, **2019**.
278. P.S. Stephanou, **V.G. Mavrantzas**, "Multiscale modeling and simulation of the viscoelasticity of

complex, microstructured fluids guided from nonequilibrium thermodynamics", *2019 Sustainable Industrial Processing Summit & Exhibition (2019 SIPS), Vayenas International Symposium*, Coral Beach Resort, Paphos, Cyprus, October 23-27, **2019**.

279. E.N. Skountzos, D.G. Tsalikis, P.S. Stephanou, **V.G. Mavrantzas**, "Atomistic simulations combined with advanced modelling for the prediction of the microscopic dynamics of polymer nanocomposites", *5th Workshop of Graduates and Post-Docs in Chemical Engineering Sciences*, Patras, Greece, November 06, **2019**.
280. K.K. Karadima, **V.G. Mavrantzas**, S.N. Pandis, "Morphology of multicomponent organic nanoaerosol", *5th Workshop of Graduates and Post-Docs in Chemical Engineering Sciences*, Patras, Greece, November 06, **2019**.
281. K.S. Karadima, **V.G. Mavrantzas**, S.N. Pandis, "Molecular Dynamics Simulation of the Microscopic Structure and Properties of Atmospheric Nanoaerosols and of the Organic Compounds Making them Up", *European Virtual Workshop on Molecular Simulations of Atmospheric Systems*, EPFL, Lausanne, June 2-4, **2020**.
282. E.N. Skountzos, K.S. Karadima, **V.G. Mavrantzas**, "Molecular simulations combined with theoretical modelling for understanding the microscopic dynamics and shear rheology of unentangled polymer nanocomposite melts", *1st Annual European Rheology Conference in Cyberspace (AERC 2021 in Cyberspace)*, April 13-15, **2021**.
283. E.N. Skountzos, K.S. Karadima, **V.G. Mavrantzas**, "The role of end groups in the structure and microscopic dynamics of unentangled poly(ethylene glycol) - silica nanocomposite melts: Simulation and Theory", *MRS Spring Meeting (Virtual)*, April 17-23, **2021**.
284. E.N. Skountzos, D.G. Tsalikis, P.S. Stephanou, **V.G. Mavrantzas**, "Coupling theory and simulations to fully elucidate the important role of end groups in poly(ethylene glycol) - silica nanocomposite melts", *Complex Fluids in Manufacturing Workshop (CORAL 2021)*, The British Society of Rheology, April 21, **2021**.
285. E.N. Skountzos, D.G. Tsalikis, P.S. Stephanou, **V.G. Mavrantzas**, "Reconciliation of experiments and theory in poly(ethylene glycol) - silica nanocomposite melts", *1st European University of Technology Workshop on Nanomaterials and Nanotechnologies (1st EUt+)*, April 28-29, **2021**.
286. P.V. Alatas, **V.G. Mavrantzas**, H.C. Öttinger, "Third-order perturbation expansion and symbolic calculation of the two-point correlation function of the dissipative quantum φ^4 theory", *Joint European Thermodynamics Conference (JETC 2021)*, Prague, Czech Republic, June 14-18, **2021**.
287. D.G. Tsalikis, **V.G. Mavrantzas**, S.E. Pratsinis, "Dynamics of molecular collisions in air beyond the kinetic theory", *European Aerosol Science Conference 2021 (EAC 2021)*, August 30-September 03, **2021**.
288. D.G. Tsalikis, **V.G. Mavrantzas**, S.E. Pratsinis, "Mechanics of molecular collisions in air from detailed molecular dynamics simulations", *EMLG/JMLG Virtual Workshop on Molecular Characterization of Interfaces in Atmospheric Aerosol*, September 13, **2021**.
289. P.G. Mermigkis, K.S. Karadima, **V.G. Mavrantzas**, S.N. Pandis, "Free Volume Analysis of Aerosol Nanoparticles", *EMLG/JMLG Virtual Workshop on Molecular Characterization of Interfaces in Atmospheric Aerosol,* September 13, **2021**.
290. P.G. Mermigkis, **V.G. Mavrantzas**, "Clusters of free volume accessible to small penetrants and their connectivity in polymer nanocomposites containing carbon nanotubes through a geometric analysis", *13th Hellenic Polymer Siociety Conference (ELEP 2021, virtual event),* Athens, Greece, December 12-16*,* **2021**.
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293. T. Alexiou, **V.G. Mavrantzas**, D. Mintis, "Molecular Dynamics simulation of the formation of polycation-based DNA complexes intended for gene delivery applications", *13th Hellenic Polymer Siociety Conference (ELEP 2021, virtual event),* Athens, Greece, December 12-16*,* **2021**.

294. D.G. Tsalikis, T.S. Alexiou, P.V. Alatas, V.G. Mavrantzas, "on the role of molecular architecture in polymer size and diffusion: The case of ring and linear poly(ethylene oxide) chains in aqueous solutions", *13th Hellenic Polymer Siociety Conference (ELEP 2021, virtual event),* Athens, Greece, December 12-16*,* **2021**.
295. T. Alexiou, D. Tsalikis, P. Stephanou, **V.G. Mavrantzas**, "Conformation and dynamics of short linear and ring DNA molecules in the crossover from the dilute to the semi-dilute solution regime: Insights from atomistic molecular dynamics simulations", *13th Hellenic Polymer Siociety Conference (ELEP 2021, virtual event),* Athens, Greece, December 12-16*,* **2021**.
296. V.-M. Nikiforidis, D.G. Tsalikis, P.S. Stephanou, V.G. Mavrantzas, "On the relationship between stress and conformation tensors in state-of-the-art constitutive models for polymer melts and the possible additional role of chain tumbling", *Annual European Rheology Conference (AERC 2022)*, Seville (Spain), April 26-28, **2022**.
297. P.V. Alatas, **V.G. Mavrantzas**, H.C. Öttinger, "Analytical calculation of the propagator of the dissipative quantum φ^4 theory up to 3rd order from nonequilibrium thermodynamics", *13th Panhellenic Chemical Engineers Conference*, Patras, Greece, June 2-4, **2022**.
298. P. Apostolaki, K.S. Karadima, **V.G. Mavrantzas**, "Study of the structure and mechanism of antimicrobial action of short peptides derived from keratin (KAMPs) using molecular dynamics simulations", *13th Panhellenic Chemical Engineers Conference*, Patras, Greece, June 2-4, **2022**.
299. P. Siachouli, K.S. Karadima, **V.G. Mavrantzas**, S.N. Pandis, "Glass transition temperature of organic compounds making up atmospheric nanoparticles from molecular dynamics simulations", *13th Panhellenic Chemical Engineers Conference*, Patras, Greece, June 2-4, **2022**.
300. **V.G. Mavrantzas**, T. Mermigkis, K.S. Karadima, S.N. Pandis, "Phase state of atmospheric nanoparticles: Geometric analysis of the free vlume accessible to small molecules", *13th Panhellenic Chemical Engineers Conference*, Patras, Greece, June 2-4, **2022**.
301. D.G. Tsalikis, P.G. Mermigkis, Ch. Christopoulou, I. Stott, **V.G. Mavrantzas**, "Salt concentration effects on the morphology of micellar solutions of ionic surfactants and their mixtures with zwitteronic co-surfactants", *13th Panhellenic Chemical Engineers Conference*, Patras, Greece, June 2-4, **2022**.
302. P.S. Stephanou, P. Vafeas, **V.G. Mavrantzas**, "A constitutive model from non-equilibrium thermodynamics for soft-soft nanocomposites", *10th International Meeting of the Hellenic Society of Rheology (HSR 2022)*, Skiathos, Greece, June 29-July 2, **2022**.
303. D.G. Tsalikis, C. Christopoulou, K.S. Karadima, I.P. Stott, V.G. Mavrantzas, "Multi-scale simulation approach to morphology and microrheology of mixed surfactant-cosurfactant micellar solutions", *10th International Meeting of the Hellenic Society of Rheology (HSR 2022)*, Skiathos, Greece, June 29-July 2, **2022**.
304. P. Siachouli, K.S. Karadima, **V.G. Mavrantzas**, S.N. Pandis, "Glass transition temperatures of atmospherically relevant organic compounds from molecular dynamics", *11th International Aerosol Conference (IAC 2022)* Athens, Greece, September 4-9, **2022**.
305. K.S. Karadima, D.G. Tsalikis, **V.G. Mavrantzas**, S.E. Pratsinis, "Diffusivities of fullerene and silica nanoparticles in air from detailed molecular dynamics", *11th International Aerosol Conference (IAC 2022)* Athens, Greece, September 4-9, **2022**.
306. K.S. Karadima, **V.G. Mavrantzas**, S. Pandis, "Diffusivity and viscosity of organic aerosol components from detailed molecular dynamics simulations", *11th International Aerosol Conference (IAC 2022)* Athens, Greece, September 4-9, **2022**.
307. P.S. Stephanou, D.G. Tsalikis, Ch. Christopoulou, **V.G. Mavrantzas**, "Variable entanglement density constitutive rheological model from nonequilibrium thermodynamics and comparison with atomistic simulation data under flow", *European Topology Interdisciplinary Action (EUTOPIA)*, Trento, Italy, September 6-9, **2022**.
308. A.J. Tsamopoulos, A.F. Katsarou, D.G. Tsalikis, **V.G. Mavrantzas**, "Shear rheology of ring polymer melts through nonequilibrium molecular dynamics simulations", *14th European Fluid Mechanics Conference*, Athens, Greece, September 13-16, **2022**.
309. K.S. Karadima, D.G. Tsalikis, I. P. Stott, **V.G. Mavrantzas**, "Salt effects on the morphology and rheology of micellar solutions of ionic surfactants through molecular simulations across scales", *14th European Fluid Mechanics Conference (EFMC14)*, Athens, Greece, September 13-16, **2022**.
310. D.G. Tsalikis, **V.G. Mavrantzas**, S.E. Pratsinis, "Dynamics of molecular collisions in air beyond

the kinetic theory", *9th World Congress on Particle Technology (WCPT-9)*, Madrid, Spain, September 18-22, **2022**.

311. K.S. Karadima, D.G. Tsalikis, **V.G. Mavrantzas**, S.E. Pratsinis, "Fullerene and silica nanoparticle diffusivities in air from molecular dynamics simulations", *9th World Congress on Particle Technology (WCPT-9)*, Madrid, Spain, September 18-22, **2022**.
312. E.N. Skountzos, D.G. Tsalikis, P.S. Stephanou, **V.G. Mavrantzas**, "A combined theoretical-simulation approach to microstructure and dynamics of poly(ethylene glycol) - silica nanocomposite melts", *5th International Conference on Structural Nano Composites (NANOSTRUC 2023)*, Nicosia, Cyprus, May 23-26, **2023**.
313. K.S. Karadima, D.G. Tsalikis, V.G. Mavrantzas, S.E. Pratsinis, "Molecular dynamics simulations of fullerene and silica nanoparticles diffusion coefficients in air", 26th ETH Nanoparticles Conference, ETH Zurich, Switzerland, June 20-22, **2023**.
314. L.D. Peristeras, K.S. Karadima, D.G. Tsalikis, I.P. Stott, **V.G. Mavrantzas**, "Brownian Dynamics simulation of the viscoelasticity of wormlike micellar solutions", *XIXth International Congress on Rheology (ICR2023)*, Athens, Greece, July 29 – August 4, **2023**.
315. D.G. Tsalikis, **V.G. Mavrantzas**, "Microscopic dynamics of long polymer ring melts from atomistic simulations and comparison with neutron spic echo measurements", *XIXth International Congress on Rheology (ICR2023)*, Athens, Greece, July 29 – August 4, **2023**.
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317. D.G. Tsalikis, **V.G. Mavrantzas**, S.E. Pratsinis, "Mean free path of air: The impact of inelastic molecular collisions", *European Aerosol Science Conference 2023 (EAC 2023)*, Malaga, Spain, 30 August – 03 September, **2023**.
318. D.G. Tsalikis, **V.G. Mavrantzas**, S.E. Pratsinis, "The Impact of Inelastic Collisions on the Mean Free Path in Air", *41st Annual Conference of the American Association for Aerosol Research (41st AAAR)*, Oregon, Portland, USA, October 2-76, **2023**.
319. P.S. Stephanou, D.G. Tsalikis, **V.G. Mavrantzas**, "A variable entanglement density constitutive model for polymer melts from nonequilibrium thermodynamics", *Annual European Rheology Conference (AERC 2024)*, Leeds, UK, April 9-12, **2024**.
320. D.G. Tsalikis, H. Papargyriou, **V.G. Mavrantzas**, "Segmental dynamics of poly(ethylene oxide) rings in melts slightly contaminated by linear counterparts", *Annual European Rheology Conference (AERC 2024)*, Leeds, UK, April 9-12, **2024**.
321. E.N. Skountzos, D.G. Tsalikis, P.S. Stephanou, **V.G. Mavrantzas**, "A combined theoretical-simulation approach to microscopic structure and dynamics of unentangled poly(ethylene glycol) – silica nanocomposite melts", *MecaNano's 2nd General Meeting,* Vienna, Austria, May 1-3, **2024**.
322. P. Panagopoulos-Papageorgiou, K.S. Karadima, I. Papageorgiou, **V.G. Mavrantzas**, "On the non-canonical structure of keratin-derived antimicrobial peptides (KAMPs) through molecular simulations", *14th Panhellenic Chemical Engineers Conference*, Thessaloniki, Greece, May 29-31, **2024**.
323. P. Siachouli, **V.G. Mavrantzas**, S.N. Pandis, "Quantitative relationship between structure and glass transition temperature of organic constituents of atmospheric particles", *14th Panhellenic Chemical Engineers Conference*, Thessaloniki, Greece, May 29-31, **2024**.
324. P. Panagopoulos-Papageorgiou, K.S. Karadima, I. Papageorgiou, **V.G. Mavrantzas**, "On the non-canonical structure of keratin-derived antimicrobial peptides (KAMPs) via molecular dynamics simulations", *BioExcel Summer School on Biomolecular Simulations 2024*, Pula, Sardinia, Italy, June 16-21, **2024**.
325. D.G. Tsalikis, **V.G. Mavrantzas**, S.E. Pratsinis, "A new equation for the mean free path of air", *European Aerosol Science Conference 2024 (EAC 2024)*, Tampere, Finland, August 25-30, **2024**.
326. P. Siachouli, **V.G. Mavrantzas**, S.N. Pandis, "Predicting & Parameterizing the Glass Transition Temperature of Atmospheric Organic Compounds via Molecular Dynamics Simulations", *4th FORTH Retreat*, Ancient Olympia, Greece, October 11-13, **2024**.
327. G. Leonis, L.D. Peristeras, **V.G. Mavrantzas**, "Antimicrobial Action of Essential Oils and CuO Nanoparticles Against Pathogenic Proteins: Elucidation of the Inhibitory Mechanism through

Molecular Dynamics and Free Energy Calculations", *2nd BioExcel Conference on Advances in Biomolecular Simulations*, Brno, Czech Republic, October 20-23, **2024**.

328. P. Panagopoulos Papageorgiou, K.S. Karadima, I. Papageorgiou, **V.G. Mavrantzas**, "Molecular dynamics simulation of keratin-derived antimicrobial peptides (KAMPs) in solution and of their interaction with bacterial membranes", *2nd BioExcel Conference on Advances in Biomolecular Simulations*, Brno, Czech Republic, October 20-23, **2024**.
329. K.S. Karadima, D.G. Tsalikis, **V.G. Mavrantzas**, S.E. Pratsinis, "Diffusivity of Small (< 10 nm) Nanoparticles in Air by Fully Atomistic Molecular Dynamics", *42nd Annual Conference of the American Association for Aerosol Reseacrch (AAAR 2024)*, Albuquerque, New Mexico, USA, October 21-25, **2024**.
330. D.G. Tsalikis, **V.G. Mavrantzas**, S.E. Pratsinis, "A new equation for the mean free path of air", *AIChE Annual Meeting (AIChE 2024)*, San Diego, USA, October 27-31, **2024**.
331. K.S. Karadima, D.G. Tsalikis, **V.G. Mavrantzas**, S.E. Pratsinis, "Diffusion coefficients of fullerene and silica nanoparticles (<10 nm) in air by fully atomistic molecular dynamics", *AIChE Annual Meeting (AIChE 2024)*, San Diego, USA, October 27-31, **2024**.
332. D.G. Tsalikis, **V.G. Mavrantzas**, S.E. Pratsinis, "Dynamics of molecular collisions in air and its mean free path", *AIChE Annual Meeting (AIChE 2024)*, San Diego, USA, October 27-31, **2024**.
333. D.G. Tsalikis, H. Papargyriou, **V.G. Mavrantzas**, "Segmental dynamics of poly(ethylene oxide) rings in melts slightly contaminated with linear analogues", *AIChE Annual Meeting (AIChE 2024)*, San Diego, USA, October 27-31, **2024**.
334. D.G. Tsalikis, **V.G. Mavrantzas**, "Shear-rate dependent viscometric functions of polymer melts from atomistic molecular dynamics", *Annual European Rheology Conference (AERC 2025)*, Lyon-France, April 14-17, **2025**.
335. D. Aslanis, L.D. Peristeras, I.P. Stott, **V.G. Mavrantzas**, "Hybrid Brownian Dynamics – kinetic Monte Carlo simulations of wormlike micellar solutions", *Annual European Rheology Conference (AERC 2025)*, Lyon-France, April 14-17, **2025**.
336. D.G. Tsalikis, **V.G. Mavrantzas,** S.E. Pratsinis, "A new (?) kinetic theory of gases and the diffusivity of tiny (< 5 nm) SiO_2 nanoparticles, *13th Mediterranean Combustion Symposium (MCS2025)*, Corfu, Greece, June 1-5, **2025**.
337. **V.G. Mavrantzas**, "Relativistic hydrodynamics from the generalized bracket formalism of non-equilibrium thermodynamics", *10th International Workshop on Non-Equilibrium Thermodynmics (IWNET 2025)*, Syros Island, Greece, June 8-11, **2025**.
338. D. Aslanis, L.D. Peristeras, I.P. Stott, **V.G. Mavrantzas**, "A combined Brownian Dynamics - kinetic Monte Carlo framework for simulating the viscoelasticity of wormlike micellar solutions", *11th International Meeting of the Hellenic Society of Rheology (HSR 2025)*, Syros Island, Greece, June 11-14, **2025**.
339. D.G. Tsalikis, **V.G. Mavrantzas**, "Shear-rate dependent viscometric functions of polymer melts from atomistic molecular dynamics", *11th International Meeting of the Hellenic Society of Rheology (HSR 2025)*, Syros Island, Greece, June 11-14, **2025**.
340. D.G. Tsalikis, **V.G. Mavrantzas,** "Probing polymer structure and dynamics through molecular dynamics simulations and comparison with NSE and SANS spectra", *Polarisation Analysed QENS: Modelling and Data Analzsis (PAQMAN)*, Stavanger, Norway, July 2-4, **2025**.
341. K.S. Karadima, D.G. Tsalikis, **V.G. Mavrantzas**, S.E. Pratsinis, "The diffusivity of nanoparticles in the free molecule regime", *European Aerosol Science Conference 2025 (EAC 2025)*, Lecce, Italy, August 31 - September 05, **2025**.
342. D.G. Tsalikis, **V.G. Mavrantzas**, S.E. Pratsinis, "Diffusion dynamics of tiny SiO2 nanoparticles in air", *European Aerosol Science Conference 2025 (EAC 2025)*, Lecce, Italy, August 31 - September 05, **2025**.
343. P. Siachouli, **V.G. Mavrantzas**, S.N. Pandis, "Predicting and parameterizing the glass transition temperature of atmospheric organic components via molecular dynamics simulations", *European Aerosol Science Conference 2025 (EAC 2025)*, Lecce, Italy, August 31 - September 05, **2025**.
344. G. Leonis, I. Papageorgiou, P. Panagopoulos Papageorgiou, L. Peristeras, K.S. Karadima, **V.G. Mavrantzas**, "Insights into the interaction of pathogens with keratin-derived antimicrobial peptides and essential oils from molecular simulations", *The 10th edition of the Smart Materials & Surfaces conference (SMS 2025)*, Rome, Italy, October 19-21, **2025**.

345. Y. Ming, **V.G. Mavrantzas**, A. Güntner, "Enhanced Molecular Sensitivity of Metastable ε-WO_3: Insights from Experiments and First-Principles Calculations", *AIChE Annual Meeting (AIChE 2025)*, Boston, USA, November 2-6, **2025**.
346. A. Spyridakis, J. Tsamopoulos, P.S. Stephanou, **V.G. Mavrantzas**, F. Simopoulos, L. Tzounis, "Tensile properties of thermoplastic polyurethane (TPU) / carbon nanotube (CNT) nanocomposites for 3D printing through experiments and simulations", *15th Hellenic Polymer Siociety Conference (ELEP 2025),* Patras, Greece, December 3-6*,* **2025**.
347. I. Papageorgiou, K.S. Karadima, L. Peristeras, **V.G. Mavrantzas**, "Encapsulation of essential oils in silica nanopores: A Molecular Dynamics simulation study", *Surfaces, Interfaces and Coatings Technologies International conference (SICT 2026),* Prague, Czech Republic, May 6 - 8, **2026**.
348. I. Papageorgiou, K.S. Karadima, **V.G. Mavrantzas**, "Study of the encapsulation and mobility of essential oils within nanoporous silica through molecular dynamics simulations", *15th Panhellenic Chemical Engineers Conference*, Chania, Greece, June 03-051, **2026**.
349. E. Petlis, L. Peristeras, G. Vogiatzis, **V.G. Mavrantzas**, "Microstructure and rheological properties of polyethylene oxide melts through coarse-grained Brownian Dynamics simulations", *15th Panhellenic Chemical Engineers Conference*, Chania, Greece, June 03-051, **2026**.
350. P. Siachouli, **V.G. Mavrantzas**, S.N. Pandis, "The self-diffusion coefficient of atmospheric organic aerosol components: A molecular dynamics simulation study", *15th Panhellenic Chemical Engineers Conference*, Chania, Greece, June 03-051, **2026**.

SELECTED – ACCEPTED 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. "*Simulation of polymers with a non-linear molecular architecture*", ΕΚΕΤΑ-ΙΤΧΗΔ, February 3, **2006**.
12. "*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**.
13. *"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.**
14. *"Polymer melt viscoelasticity: What can we learn from molecular simulations",* Department of

Materials Science, University of Crete, Heraklion, Crete, May 25, **2007**.

15. *"Polymer melt viscoelasticity: What can we learn from molecular simulations",* Department of Applied Physics, University of Eindhoven, Eindhoven, The Netherlands, October 1, **2007**.
16. *"Hierarchical Modeling of Polymers: From the atomistic to the meso- to the macro-scale",*ENPC, Paris, November 26, **2007**.
17. *"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**.
18. *"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.**
19. *"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**.
20. "*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**.
21. "*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**.
22. "*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**.
23. *"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**.
24. *"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**.
25. *"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**.
26. *"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**.
27. *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.**
28. *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**.
29. *Atomistic Monte Carlo simulation of self-assembly in soft matter systems,* SCIMEETING Europe, Materials Modellig and Simulations Conference, Athens, Greece, June 21-23, **2017**.
30. *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**.
31. *Microscopic dynamics and threadings in ring polymers: A detailed computer simulation study*, Ring Polymers: Focused Workshop*,* Heraklion, Crete, September 25-27, **2017**.
32. *Molecular modelling of materials: making a difference in industry,* Plastics Update, 2nd edition, Fribourg, Switzerland, November 9, **2017**.
33. *Multiscale materials modelling with emphasis to polymers: making a difference in industry,* International Workshop on Smart Models for Smart Materials $(SM)^2$, March 27-28, Fraunhofer-Zentrum, Kaiserslautern, **2019**.
34. *Topological Interactions in melts of ring polymers and their effect on dynamic and rheological*

*proeprties***.** 13th Hellenic Polymer Siociety Conference (ELEP 2021, virtual event), Athens, Greece, December 12-16, **2021**.

35. *Symbolic calculation of multi-time correlation functions in dissipative φ^4 quantum field theory*. Symposium on the occasion of the retirement of Hans Christian Öttinger from the chair of Polymer Physics, Department of Materials, ETH Zurich, Switzerland, January 27, **2023**.
36. *The key role of threading events in the dynamics of polymer ring melts,* CECAM meeting on "Ring Polymer Dynamics", Prato, Italy, June 19-24, **2023**.
37. *Topological constraints and microscopic dynamics in melts of ring polymers*, JNNFM-JoR-RA on-line seminar series, April 17, **2024**.

TEACHING

Undergraduate Courses

1. "*Physical Chemistry*", Department of Chemical Engineering, University of Patras: Fall **2017** (with Prof. D. Kondarides), Fall **2018** (with Prof. D. Kondarides), Fall **2019** (with Prof. D. Kondarides), Fall **2020** (with Prof. D. Kondarides), Fall **2021** (with Prof. D. Kondarides), Fall **2022** (with Prof. D. Kondarides), Fall **2023** (with Prof. D. Kondarides), Fall **2024** (with Prof. D. Kondarides), Fall **2025** (with Prof. D. Kondarides), Fall **2026** (with Prof. D. Kondarides).
2. "*Technical Thermodynamics and Balances*", Department of Chemical Engineering, University of Patras: Fall **2019** (with Prof. D. Spartinos), Fall **2020** (with Prof. D. Vagenas), Fall **2021** (with Prof. A. Armaou), Fall **2022** (with Prof. A. Armaou), Fall **2023** (with Prof. A. Armaou), Fall **2024** (with Prof. A. Armaou), Fall **2025** (with Prof. A. Armaou), Fall **2026** (with Prof. A. Armaou).
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. *"Polymer rheology"*, Department of Chemical Engineering, University of Patras: Fall **2006**, Fall **2007**, Fall **2008,** Fall **2009**, Fall **2010**, Fall **2011**, Fall **2012**.
5. "*Special Topics of Physical Chemistry*", Department of Chemical Engineering, University of Patras: Fall **2003**, Fall **2004**, Fall **2005**.
6. "*Introduction to informatics I*", Laboratory, Department of Materials Science, University of Patras: Fall **2000** (with Dr. A. Terzis, Dr. E. Serpi, Dr. A. Vanakaras).
7. "*Introduction to informatics II*", Department of Materials Science, University of Patras: Spring **2002** (with Dr. A. Vanakaras, and Dr. M. Paspalakis).

Graduate Courses

1. *Diffusional Operations,* Department of Chemical Engineering, University of Patras: Spring **2021** (with Prof. A. Armaou), Spring **2022** (with Prof. A. Armaou), Spring **2023** (with Prof. A. Armaou), Spring **2024** (with Prof. A. Armaou), Spring **2025** (with Prof. A. Armaou), Spring **2026** (with Prof. A. Armaou).
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**, Spring **2019**.
3. "*Polymer rheology*", Inter-departmental Programme of Graduate Studies on "Science and Technology of Polymers and Composite Materials", 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), Fall **2018** (with Dr. D.G. Tsalikis), Fall **2019** (with Dr. D.G. Tsalikis), Fall **2020** (with Dr. D.G. Tsalikis), Fall **2021** (with Dr. D.G. Tsalikis), Fall **2022** (with Dr. D.G. Tsalikis), Fall **2023**, Fall **2024**, Fall **2025,** Fall **2026** (with Prof. G. Vogiatzis).
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. "*Computer simulation of polymers*", Interdepartmental Programme of Graduate Studies on "Science and Technology of Polymers and Composite Materials", University of Patras: Spring **1999,** Spring **2000,** Spring **2002** (with Dr. A. Terzis and Prof. D. Theodorou).
6. "*Polymer rheology and processing*", Inter-departmental Programme of Graduate Studies on "Science and Technology of Polymers and Composite Materials", University of Patras: Fall **2000**, Spring **2002** (with Prof. J. Tsamopoulos).

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)*
    - Fall **2016** (with Prof. S.E. Pratsinis, Lectures: 43%)
    - Fall **2017** (with Prof. S.E. Pratsinis, Lectures: 93%)
    - Fall **2018** (with Prof. S.E. Pratsinis, Lectures: 80%)
    - Fall **2019** (with Prof. S.E. Pratsinis, Lectures: 80%, Homeworks: 65%)

2. *Micro- & Nano-Particle Technology (MNP)*
    - Fall **2020** (with Prof. S.E. Pratsinis, Homeworks: 20%)
    - Fall **2021** (with Prof. S.E. Pratsinis, Homeworks: 20%)
    - Fall **2022** (with Prof. S.E. Pratsinis, Homeworks: 80%)
    - Fall **2023** (with Prof. S.E. Pratsinis, Homeworks: 80%)

3. *Mass Transfer (MT)*
    - Fall **2018** (with Prof. S.E. Pratsinis, Lectures: 20%)
    - Fall **2019** (with Prof. S.E. Pratsinis, Lectures: 20%)
    - Fall **2020** (with Prof. S.E. Pratsinis, Lectures: 60%, Homeworks: 20%)
    - Fall **2021** (with Prof. S.E. Pratsinis, Lectures: 45%, Homeworks: 70%)
    - Fall **2022** (with Prof. S.E. Pratsinis and C.-J. Shih, Lectures: 45%, Homeworks: 70%)
    - Fall **2023** (with Profs. S.E. Pratsinis, A. Güntner and C.-J. Shih, Lectures: 45%, Homeworks: 70%)
    - Fall **2024** (with Profs. M. Tibbitt and C.-J. Shih, Lectures: 55%, Homeworks: 70%)
    - Fall **2025** (with Profs. M. Tibbitt and C.-J. Shih, Lectures: 45%, Homeworks: 70%)
    - Fall **2026** (with Profs. M. Tibbitt and C.-J. Shih, Lectures: 45%, Homeworks: 70%)

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 (graduate in 2018)
20. Christos Georgantopoulos (graduate in 2018)
21. Eleni Chousa (graduate in 2018)
22. Alexandros Tsamopoulos (graduate in 2019)
23. Despoina Rigou (graduate in 2019)
24. Anna Katsarou (graduate in 2019)
25. Evaggelia Kriti (graduated in 2019)
26. Aspasia Triantafyllou (graduated in 2020)
27. Dimitris Loukas (graduated in 2021)
28. Panagiotis Kargados (graduated in 2021)
29. Christina Christopoulou (graduated in 2021)
30. Alexandros Koulouris (graduated in 2021)
31. Alexandros Priovolos (graduated in 2021)
32. Anna Tsala (graduated in 2021)
33. Anastasia Mavragani (graduated in 2021)
34. George Benakis (graduated in 2022)
35. Pinelopi Apostolaki (graduated in 2022)
36. Maria-Anna Antoniou (graduated in 2022)
37. Katerina Laskari (graduated in 2023)
38. Panagiotis Panagopoulos-Papageorgiou (graduated in 2023)
39. Ioanna Papagergiou (graduated in 2023)
40. Haris Papargyriou (graduated in 2024)
41. Georgios Ntamptsis (graduated in 2024)
42. Dimitra Ragiou (2020 – to date)
43. Alexandros Tsatsoulis (graduated in 2025)
44. George Perdikouris (graduated in 2025)
45. Lefteris Rasidakis (graduated in 2026)
46. Efi Lepenioti (graduated in 2026)
47. Aristeidis Koukoutsis (graduated in 2026)
48. Athina Spyropoulou (2025 – to date)
49. Konstantina Charami (2025 – to date)
50. George Athanasopoulos (2025 – 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 (graduated in 2018)
10. Ioanna Tsimouri (graduated in 2018)
11. Evangelos Petlis (graduated in 2026)

Ph.D. students

1. Katerina Foteinopoulou (jointly with Profs. 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. Flora Tsourtou (graduated in 2019)
7. Dimitris Mintis (graduated in 2020)
8. Emmanouil Skountzos (graduated in 2022)
9. Takis Mermigkis (graduated in 2022)
10. Panagiotis Alatas (graduated in 2023)
11. Nota Siachouli (graduated in 2025) (jointly with Prof. S.N. Pandis)
12. Ioanna Papageorgiou (2023 – to date)

Post-Doctoral and Senior 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. Alexandros Anastassiou (2013)
8. Orestis Alexiadis (2009 – 2014)
9. Dimitrios Tsalikis (2011 – to date)
10. Katerina Karadima (2013 – to date)
11. Pavlos Stephanou (2017 – 2019)
12. Stavros Peroukidis (2017 – 2020)
13. Terpsichori Alexiou (2017 – 2021)
14. Emmanouil Symianakis (2018 – 2020)
15. George Leonis (2023 – 2026)

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

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)
3. Simon Benz (academic advisor: Prof. S.E. Pratsinis, graduated in 2019)
4. Max Kroppen (academic advisor: Prof. S.E. Pratsinis, graduated in 2021)
5. Jonas Hildebrandt (academic advisor: Prof. S.E. Pratsinis, graduated in 2025)
6. Jamie Geiss (academic advisor: Prof. Mark Tibbitt)

Masters' Degree students

1. Vasil Vasilev (academic advisor: Prof. S.E. Pratsinis, graduated in 2017)
2. Max Kroppen (academic advisor: Prof. S.E. Pratsinis, graduated in 2023)

Ph.D. students

1. Anastasia Spyrogianni (co-advised with Prof. S.E. Pratsinis, graduated in 2017)
2. Alexander Weyman (co-advised with Prof. H.C. Öttinger, graduated in 2022)

Post-Doctoral Collaborators

1. Dr. Nikolaos Lempesis (co-advised with Prof. S.E. Pratsinis, 2017 - 2018)
2. Dr. Katerina Karadima (co-advised with Prof. S.E. Pratsinis, 2022 - 2024)
3. Dr. Dimitrios Tsalikis (co-advised with Prof. S.E. Pratsinis, 2023 - 2025)

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. Co-chair, 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. Chair, Organizing and Scientific Committee, *4th International Workshop on Non-equilibrium Thermodynamics and Complex Fluids (IWNET 2006),* 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 IWNNFM 2007),* 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. Chair, Organizing and Scientific Committee, Focused Workshop on Self-Assembly in Soft matter, Patras, Greece, Sept. 10-14, **2014**. The GENESIS Workshop.
12. Member, Organizing and Scientific Committee, *7th International Workshop on Non-equilibrium Thermodynamics and Complex Fluids (IWNET 2015),* Hilvarenbeek, The Netherlands, July 6-10, **2015**.

13. Member, Scientific Committee, *European Polymer Gongress (EPF 2019),* Heraklion, Crete, Greece, June 9-14, **2019**.
14. Member, Scientific Committee, *9th International Conference of the Hellenic Society of Rheology*, Samos, Greece, June 23-27, **2019** (Conference dedicated to Prof. Gary L. Leal).
15. Member, Scientific Committee, *International Conference on Adhesion in Aqueous Media: From Biology to Synthetic Materials (AAM 2019)*, Hilton Dresden, Germany, September 9-12, **2019**.
16. Member, Scientific Committee, *3rd International Meeting of the Hellenic Society of Rheology*, Patras, Greece, June 30 – July 02, **2022** (Conference dedicated to Prof. Giuseppe Marrucci and Evan Mitsoulis).
17. Member, Local Organizing Committee, *ΙΘ' International Congress on Rheology (ICR 2023),* Athens, Greece, July 29 - August 04, **2023**.
18. Co-chair, Organizing Committee, *10th International Workshop on NonEquilibrium Thermodynamics (IWNET 2025)*, Syros, Greece, June 08-June 11, **2025** (Conference dedicated to Prof. Miroslav Grmela).
19. Co-chair, Organizing and Scientific Committee, *11th International Meeting of the Hellenic Society of Rheology*, Syros, Greece, June 11-14, **2025** (Conference dedicated to Prof. Masao Doi).

SERVICES, DEPARTMENT OF CHEMICAL ENGINEERING, UNIVERSITY OF PATRAS

1. Seminars Committee
   - Chair: 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
   - Chair: 2021 - to date
3. Committee of Graduate Studies, Chairman, 2007-2009
   - Member: 2005-2007, 2024-to date
   - Chair: 2007-2009, 2009-2011, 2011-2014, 2017-2024
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

Em. Prof. Hans Christian Öttinger
Department of Materials
ETH-Zürich
CH-8093 Zürich
Switzerland
e-mail: hco@mat.ethz.ch
tel.: +41 1 632 3127

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

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

Em. Prof. Sotiris E. Pratsinis
Departmnet of Mechanical and Process Engineering
ETH-Zürich
CH-8092 Zürich
Switzerland
e-mail: sotiris.pratsinis@mavt.ethz.ch
tel.: +41 44 632 31 80

Prof. Dimitris Vlassopoulos
Department of Materials Science
University of Crete & FORTH-IESL

Prof. Spyros Pandis
Department of Chemical Engineering
University of Patras

Heraklion, Crete 70013
Greece
e-mail: dvlasso@iesl.forth.gr
tel.: +30 2810 391469

Patras, GR 26500
Greece
email: spyros@chemeng.upatras.gr
tel.: +30 2610 969510