VLASIS G. MAVRANTZAS

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ETH Zürich
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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
- 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

Lecturer (September 2016- today)
Department of Mechanical and Process Engineering, 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)

DISTINCTIONS

- Section Editor-in-Chief, Polymer Physics, *Polymers*, MDPI (since 2020).

- 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, 2-4 June, **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, 2-4 June, **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)
- Secretary, Hellenic Society of Rheology (HSR)

ADMINISTRATIVE POSITIONS

- Secretary-Treasurer, Hellenic Society of Rheology (HSR), September 2006-to date
- President of the Hellenic Society of Rheology (HSR), September 2004-September 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

INDUSTRIAL PROJECTS

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

PROPOSALS FOR CPU TIME

1. "*Large scale atomistic simulations of ring polymer melts: understanding the origin of slow relaxation modes (NaNoComp)*", CPU Research Grant, Greek Research & Technology Network (GRNET), National HPC facility – ARIS, Project No pr001030, CPU time granted: 1,951,200 core hours, **October2015**.
2. "*Large scale atomistic simulations of ring polymer melts: understanding the origin of slow relaxation modes (RingProbes)*", CPU Research Grant, Greek Research & Technology Network (GRNET), National HPC facility – ARIS, Project No pr006050, CPU time granted: 1,951,200 core hours, **May 2016**.
3. "*Large-scale molecular dynamics simulations of the phenomenon of complex coacervation (COACERVATE)*", CPU Research Grant, Greek Research & Technology Network (GRNET), National HPC facility – ARIS, Project No pr004011, CPU time granted: 1,520,640 core hours, **May 2017**.
4. "*Molecular dynamics simulation of multicomponent atmospheric nanoparticles: understanding the role of organic compound type and relative humidity in particle's structure (AtmoStruc)*", CPU Research Grant, Greek Research & Technology Network (GRNET), National HPC facility – ARIS, Project No pr004005, CPU time granted: 1,512,000 core hours, **May 2017**.
5. "*Large-scale molecular dynamics simulations of the phenomenon of complex coacervation, Phase II (COACERVATE II)*", CPU Research Grant, Greek Research & Technology Network (GRNET), National HPC facility – ARIS, Project No pr006050, CPU time granted: 3,412,115 core hours,

October 2017.

6. "*Large scale computer simulations for the exploration of the sequence of phase transitions and dynamics of poly- and oligo-thiophenes (ThioSim)*", CPU Research Grant, Greek Research & Technology Network (GRNET), National HPC facility – ARIS, Project No pr005043, CPU time granted: 2,211,840 core hours, **October 2017**.
7. "*Molecular dynamics simulation or DNA rings (RingDNA)*", CPU Research Grant, Greek Research & Technology Network (GRNET), National HPC facility – ARIS, Project No pr002038, CPU time granted: 1,520,640 core hours, **October 2017**.
8. *"Diffusivity measurements of organics in multicomponent organic aerosols via large-scale molecular dynamics simulations (DiffOA)*", CPU Research Grant, Greek Research & Technology Network (GRNET), National HPC facility – ARIS, Project No pr006017, CPU time granted: 1,200,000 core hours, October 2018.
9. "*Large-scale molecular dynamics simulations of weak polyelectrolytes: towards the development of bio-inspired materials with tunable adhesion (CoaBrush_I)*", CPU Research Grant, Greek Research & Technology Network (GRNET), National HPC facility – ARIS, Project No pr006011, CPU time granted: 3,374,432 core hours, **May 2018**.
10. "*Hierarchical modeling and simulation of sodium dodecyl sulfate (SDS)-based aqueous solutions (HieraMod)*", CPU Research Grant, Greek Research & Technology Network (GRNET), National HPC facility – ARIS, Project No pr006050, CPU time granted: 3,594,600 core hours, **May 2018**.
11. "*Molecular dynamics simulations of polymersome constructed from di-block linear copolymers of poly(ethylene glycol) (PEG) and polystyrene (PS) (PolyMplex)*", CPU Research Grant, Greek Research & Technology Network (GRNET), National HPC facility – ARIS, Project No pr006050, CPU time granted: 3,594,600 core hours, **May 2019**.
12. "*Large-scale molecular dynamics simulations of synthetic biocompatible nano-vesicles: two case studies for a) the removal of endogenous ammonia toxins, and b) the encapsulation of polycation-based DNA complexes for gene delivery– phase II*", CPU Research Grant, Greek Research & Technology Network (GRNET), National HPC facility – ARIS, Project No ???, CPU time granted: 3,594,600 core hours, **October 2019**.
13. *"The role of amines in the structure of organic atmospheric nanoaerosols (AminONano)"*, CPU Research Grant, Greek Research & Technology Network (GRNET), National HPC facility – ARIS, Project No 8004, CPU time granted: 2,000,000 core hours, **October 2019**.

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.
45. K. Foteinopoulou, N.Ch. Karayiannis, **V.G. Mavrantzas**, M. Kröger,* "Primitive path identification and entanglement statistics in polymer melts: Results from direct topological analysis on atomistic polyethylene models", *Macromolecules* **2006**, *39*, 4207-4216.
46. O. Alexiadis, V.A. Harmandaris,* **V.G. Mavrantzas**, L. Delle Site, "Atomistic simulation of

alkanethiol self-assembled monolayers on different metal surfaces via a quantum, first-principles parametrization of the sulfur-metal interaction", *J. Phys. Chem. C'* **2007**, *111*, 6380-6391.

47. C. Baig, **V.G. Mavrantzas**,* "Thermodynamically guided nonequilibrium Monte Carlo for generating realistic shear flows in polymeric systems", *Phys. Rev. Lett.* **2007**, *99*, 257801.
48. T.C. Ionescu, B.J. Edwards,* D.J. Keffer, **V.G. Mavrantzas**, "Energetic and entropic elasticity of nonisothermal flowing polymers: Experiment, theory, and simulation ", *J. Rheol.* **2008**, *52*, 105-140.
49. O. Alexiadis, K.Ch. Daoulas, **V.G. Mavrantzas**,* "An efficient Monte Carlo algorithm for the fast equilibration and atomistic simulation of alkanethiol self-assembled monolayers on a Au(111) substrate", *J. Phys. Chem. B* **2008**, *112*, 1198-1211.
50. O. Alexiadis, **V.G. Mavrantzas**, R. Khare, J. Beckers, A.R.C. Baljon,* "End-bridging Monte Carlo simulation of bulk and grafted amorphous polyethylene above and below the glass transition", *Macromolecules* **2008**, *41*, 987-996.
51. T.C. Ionescu, B.J. Edwards,* D.J. Keffer, **V.G. Mavrantzas**, "Atomistic simulation of energetic and entropic elasticity in short-chain polyethylenes", *J. Rheol.* **2008**, *52*, 567-589.
52. G. Tsolou, V.A. Harmandaris, **V.G. Mavrantzas**,* "Molecular dynamics simulation of temperature and pressure effects on the intermediate length scale dynamics and zero shear rate viscosity of cis-1,4-polybutadiene: Rouse mode analysis and dynamic structure factor spectra", *J. non-Newt. Fluid Mech.* **2008**, *152*, 184–194.
53. G. Tsolou, **V.G. Mavrantzas**,* Z. Makrodimitri, I.G. Economou, R. Gani, "Atomistic simulation of the sorption of small gas molecules in polyisobutylene", *Macromolecules* **2008**, *41*, 6228-6238.
54. P.S. Stephanou, C. Baig, **V.G. Mavrantzas**,* "A generalized differential constitutive equation for polymer melts based on principles of non-equilibrium thermodynamics", *J. Rheol.* **2009**, 53, 309-337.
55. C. Baig,* **V.G. Mavrantzas**,* "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", *Phys. Rev. B* **2009**, *79*, 144302.
56. K.C. Satyanarayana, J. Abildskov, R. Gani,* G. Tsolou, **V.G. Mavrantzas**, "Computer-aided polymer design using multi-scale modelling", *Brazilian J. Chem. Eng.* **2010**, *27*, 369-380.
57. P.S. Stephanou, C. Baig, G. Tsolou, **V.G. Mavrantzas**,* M. Kröger, "Quantifying chain reptation in entangled polymer melts: Topological and dynamical mapping of atomistic simulation results onto the tube model", *J. Chem. Phys.* **2010**, *132*, 124904.
58. C. Baig,* **V.G. Mavrantzas**,* "Tension thickening, molecular shape, and flow birefringence of an H-shaped polymer melt in steady shear and planar extension", *J. Chem. Phys.* **2010**, *132*, 014904.
59. C. Baig, O. Alexiadis, **V.G. Mavrantzas,*** "Advanced Monte Carlo algorithm for the atomistic simulation of short- and long-chain branched polymers: Implementation for H-shaped, q-shaped, and short-chain branched polyethylene melts", *Macromolecules* **2010**, *43*, 986–1002.
60. C. Baig,* **V.G. Mavrantzas**, M. Kröger, "Flow effects on melt structure and entanglement network of linear polymers: Results from a nonequilibrium molecular dynamics simulation study of a polyethylene melt in steady shear", *Macromolecules* **2010**, *43*, 6886–6902.
61. C. Baig, **V.G. Mavrantzas**,* "From atomistic trajectories to primitive paths to tube models: Linking molecular simulations with the reptation theory for entangled polymer melts", *Soft Matter* **2010**, *6*, 4603-4612.
62. C. Baig, P.S. Stephanou, G. Tsolou, **V.G. Mavrantzas**,* M. Kröger, "Understanding Dynamics in Binary Mixtures of Entangled cis-1,4-Polybutadiene Melts at the Level of Primitive Path Segments by Mapping Atomistic Simulation Data onto the Tube Model", *Macromolecules* **2010**, *43*, 8239–8250.
63. G. Tsolou, N. Stratikis, C. Baig,* P.S. Stephanou, V.G. Mavrantzas.* "Melt Structure and Dynamics of Unentangled Polyethylene Rings: Rouse Theory, Atomistic Molecular Dynamics Simulation, and Comparison with the Linear Analogues", *Macromolecules* **2010**, *43*, 10692–10713.
64. C. Baig,* **V.G. Mavrantzas**,* H.C. Öttinger, "On Maxwell's Relations of Thermodynamics for Polymeric Liquids away from Equilibrium", *Macromolecules* **2011**, *44*, 640–646.
65. P.S. Stephanou, C. Baig,* **V.G. Mavrantzas**,* "Projection of atomistic simulation data for the dynamics of entangled polymers onto the tube theory: Calculation of the segment survival probability function and comparison with modern tube models", *Soft Matter* **2011**, *7*, 380-395.

66. P.S. Stephanou, C. Baig,* **V.G. Mavrantzas**,* "Toward an improved description of constraint release and contour length fluctuations in tube models for entangled polymer melts from detailed atomistic molecular dynamics simulation data", *Macromol. Theory & Simul.,* **2011**, *20*, 752-768.
67. A.R. Brás,* R. Pasquino, T. Koukoulas, G. Tsolou, O. Holderer, A. Radulescu, J. Allgaier, **V.G. Mavrantzas**, W. Pyckhout-Hintzen, A. Wischnewski, D. Vlassopoulos, D. Richter, "Structure and Dynamics of Polymer Rings by Neutron Scattering: Breakdown of the Rouse Model", *Soft Matter* **2011**, 7, 11169-11176.
68. J. Qin, S.T. Milner,* P.S. Stephanou, **V.G. Mavrantzas**, "Effects of tube persistence length on dynamics of mildly entangled polymers, *J. Rheology* **2012**, *56*, 707-724.
69. O. Alexiadis, **V.G. Mavrantzas***, "All-atom molecular dynamics simulation of temperature effects on the structural, thermodynamic and packing properties of the pure amorphous and pure crystalline phases of regioregular P3HT", *Macromolecules* **2013**, *46*, 2450-2467.
70. P.S. Stephanou,* **V.G. Mavrantzas**,* "Quantitative predictions of the linear viscoelastic properties of entangled polyethylene and polybutadiene melts via modified versions of modern tube models on the basis of atomistic simulation data", *J. Non-Newt. Fluid Mech.* **2013**, *200*, 111-130.
71. Anastasiou A., E.K. Karahaliou, O. Alexiadis, **V.G. Mavrantzas**,* "Detailed atomistic simulation of the nano-sorption and nano-diffusivity of water, tyrosol, vanillic acid and p-coumaric acid in single wall carbon nanotubes", *J. Chem. Phys.* **2013**, *139*, 164711.
72. D.G. Tsalikis, C. Baig, **V.G. Mavrantzas**,* E. Amanatides, D. Mataras,* "A hybrid kinetic Monte Carlo method for simulating silicon films grown by plasma-enhanced chemical vapor deposition", *J. Chem. Phys.* **2013**, *139*, 204706.
73. D.G. Tsalikis, T. Koukoulas, V.G. Mavrantzas,* "Dynamic, conformational and topological properties of ring-linear poly(ethylene oxide) blends from molecular dynamics simulations", *React. & Funct. Polym.* **2014**, *80*, 61-70.
74. P.S. Stephanou,* **V.G. Mavrantzas**,* "Accurate prediction of the linear viscoelastic properties of highly entangled mono and bidisperse polymer melts", *J. Chem. Phys.* **2014**, *140*, 214903.
75. S Tsouka, Y. Dimakopoulos, **V.G. Mavrantzas**, J. Tsamopoulos,* "Stress gradient induced migration of polymers in corrugated channels", *J. Rheol.* **2014**, *58*, 911-947.
76. P.S. Stephanou,* **V.G. Mavrantzas**,* G.C. Georgiou, "Continuum model for the phase behavior, microstructure and rheology of unentangled polymer nanocomposite melts", *Macromolecules* **2014**, *47*, 4493−4513.
77. D.G. Tsalikis, **V.G. Mavrantzas**,* "Threading of ring poly(ethylene oxide) molecules by linear chains in the melt", *ACS Macro Lett.* **2014**, *3*, 763−766.
78. E.N. 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", *Macromolecules* **2014**, *47*, 8072–8088.
79. 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", Danckwerts Special Issue, *Chemical Engineering Science* **2015**, *121*, 32-50.
80. T. Mermigkis, D.G. Tsalikis, **V.G. Mavrantzas**,* "Determination of water effective diffusivity in a poly (methyl methacrylate) membrane containing carbon nanotubes using kinetic Monte Carlo simulations", *J. Chem. Phys.* **2015**, *143*, 164903.
81. A. Anastassiou, **V.G. Mavrantzas**, "Molecular Structure and work of adhesion of poly(n-butyl acrylate) and poly(n-butyl acrylate-co-acrylic acid) on α-quartz, α-ferric oxide, and α-ferrite from detailed molecular dynamics Simulations", *Macromolecules* **2015**, *48*, 8262−8284.
82. K.D. Papadimitriou, E.N. Skountzos, S.S. Gkermpoura, I. Polyzos, **V.G. Mavrantzas**, C. Galiotis, C. Tsitsilianis,* "Molecular modelling combined with advanced chemistry for the rational design of efficient graphene dispersing agents", *ACS Macro Lett.* **2016**, *5*, 24−29.
83. P.S. Stephanou,* I.Ch. Tsimouri, **V.G. Mavrantzas**, "Flow-induced orientation and stretching of entangled polymers in the framework of non-equilibrium thermodynamics", *Macromolecules* **2016**, *49*, 3161−3173.
84. D.G. Tsalikis, **V.G. Mavrantzas**,* D. Vlassopoulos, "Analysis of slow modes in ring polymers: Threading of rings controls long-time relaxation", *ACS Macro Lett.* **2016**, *5*, 755−760.
85. G.D. Papadopoulos, 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", *Polymers (Special Issue on Semiflexible Polymers)* **2016**, *8*, 283.

86. P.V. Alatas, D.G. Tsalikis, **V.G. Mavrantzas**,* "Detailed molecular dynamics simulation of the structure and self-diffusion of linear and cyclic n-alkanes in melt and blends", *Macromolecular Theory & Simulations* (Special 25th Anniversary Issue) **2017**, *26*, 1600049.
87. D.G. Tsalikis, T. Koukoulas, **V.G. Mavrantzas**,* R. Pasquino, D. Vlassopoulos, W. Pyckhout-Hintzen, A. Wischnewski, M. Monkenbusch, D. Richter, "Microscopic structure, conformational properties and equilibrium dynamics of ring and linear polyethylene oxide (PEO) melts from detailed atomistic molecular dynamics simulations: Dependence on chain length and direct comparison with experimental data", *Macromolecules* **2017**, *50*, 2565−2584.
88. K.S. Karadima, **V.G. Mavrantzas**,* S.N. Pandis, "Molecular dynamics simulation of local concentration and structure in organic aerosol nanoparticles under atmospheric conditions", *Physical Chemistry Chemical Physics* **2017**, *19*, 16681-16692.
89. A Spyrogianni, K.S. Karadima, E. Goudeli, **V.G. Mavrantzas**,* S.E. Pratsinis,* "Mobility and settling rate of agglomerates of polydisperse nanoparticles", *J. Chem. Phys.* **2018**, *148*, 064703.
90. I. Ch. Tsimouri, P.S. Stephanou,* **V.G. Mavrantzas**, "A constitutive rheological model for agglomerating blood derived from nonequilibrium thermodynamics", *Physics of Fluids* **2018**, *30*, 030710.
91. N. Lempesis, N. Smatsi, **V.G. Mavrantzas**,* S.E. Pratsinis, "Temperature- and pressure-induced monoclinic to orthorhombic phase transition in silicalite-1", *J. Phys. Chem. C* **2018**, *122*, 6217-6229.
92. D.G. Tsalikis, P.V. Alatas, L.D. Peristeras, **V.G. Mavrantzas**,* "Scaling laws for the conformation and viscosity of ring polymers in the crossover region around M_e from detailed molecular dynamics simulations", *ACS Macro Lett.* **2018**, *7*, 916–920.
93. F.D. Tsourtou, E.N. Skountzos, S.D. Peroukidis, **V.G. Mavrantzas**,* "Molecular simulation of the high temperature phase behaviour of α-unsubstituted sexithiophene", *Soft Matter* **2018**, *14*, 8253 – 8266.
94. E.N. Skountzos, P.G. Mermigkis, **V.G. Mavrantzas**,* "Molecular dynamics study of an atactic poly(methyl methacrylate) - carbon nanotube (PMMA-CNT) nanocomposite", *J. Phys. Chem. B* **2018**, *122*, 9007-9021.
95. F.D. Tsourtou, S.D. Peroukidis, L.D. Peristeras, **V.G. Mavrantzas**,* "Monte Carlo algorithm based on internal bridging moves for the atomistic simulation of thiophene oligomers and polymers", *Macromolecules* **2018**, *51*, 8406-8423.
96. P.S. Stephanou,* D.G. Tsalikis, E.N. Skountzos, **V.G. Mavrantzas**, "Understanding the rheological behavior of polymer nanocomposites: Non-equilibrium thermodynamics modeling coupled with detailed atomistic non-equilibrium molecular dynamics simulations", *Materials Today: Proceedings* **2018**, *5*, 27589–27598.
97. S.S. Gkermpoura, K.D. Papadimitriou, E.N. Skountzos, I. Polyzos, M.G.P. Carbone, A. Kotrotsos, **V.G. Mavrantzas**, C. Galiotis, C. Tsitsilianis,* "3-Arm Star Pyrene-Functional PMMAs for efficient exfoliation of Graphite in Chloroform: Fabrication of Graphene-Reinforced Fibrous Veils", *Nanoscale* **2019**, *11*, 915-931.
98. K.S. Karadima, **V.G. Mavrantzas**, S.N. Pandis, "Insights into the morphology of multicomponent organic/inorganic aerosols from molecular dynamics simulations", *Atmos. Chem. Phys. Discuss*. **2019**, *19*, 5571-5587.
99. D.G. Mintis, **V.G. Mavrantzas**,* "Effect of pH and Molecular Length on the Structure and Dynamics of Short Poly(acrylic acid) in Dilute Solution: Detailed Molecular Dynamics Study", *J. of Physical Chemistry B* **2019**, *123*, 4204-4219.
100. **V.G. Mavrantzas**,* S.E. Pratsinis, "The impact of molecular simulations in gas-phase manufacture of nanomaterials", *Current Opinion in Chemical Engineering* **2019**, *23*, 174-183.
101. A.J. Tsamopoulos, A.F. Katsarou, D.G. Tsalikis,* **V.G. Mavrantzas**,* "Shear rheology of unentangled and marginally entangled ring polymer melts from large-scale nonequilibrium molecular dynamics simulations", *Polymers* **2019**, *11*, 1194.
102. P.G. Mermigkis, E.N. Skountzos, **V.G. Mavrantzas**,* "High polymer mass densities at the mouths of carbon nanotubes (CNTs) control the diffusion of small molecules through CNT-based polymer nanocomposite membranes," *J. Phys. Chem. B* **2019**, *123*, 6892-6900.

103. F.D. Tsourtou, S.D. Peroukidis, **V.G. Mavrantzas**,* "Molecular dynamics simulation of α-unsubstituted oligo-thiophenes: Dependence of their high-temperature liquid-crystalline phase behaviour on molecular length", *J. Mater. Chem. C* **2019**, *7*, 9984.
104. O. Alexiadis, N. Cheimarios, L.D. Peristeras, **V.G. Mavrantzas**, D.N. Theodorou, J.-R. Hill, X. Krokidis, "Chameleon: A generalized, connectivity altering software for tackling properties of realistic polymer systems", *WIREs Computational Molecular Science* **2019**, *9*, e1414.
105. T. Vasileiadis,* E.N. Skountzos, D. Foster, S.P. Coleman, D. Zahn, F. Krečinić, **V.G. Mavrantzas**, R.E. Palmer, R. Ernstorfer,* "Ultrafast rotational motions of supported nanoclusters probed by electron diffraction", *Nanoscale Horiz.* **2019**, *4*, 1164-1173.
106. D.G. Mintis, M. Dompé, M. Kamperman, **V.G. Mavrantzas**,* "Effect of polymer concentration on the structure and dynamics of short poly(N,N-dimethylaminoethyl methacrylate) in aqueous solution: A combined experimental and molecular dynamics study", *J. Phys. Chem. B* **2020**, *124*, 240-252.
107. D.G. Tsalikis, **V.G. Mavrantzas**,* "Size and diffusivity of polymer rings in linear polymer matrices: The key role of threading events", *Macromolecules* **2020**, *53*, 803-820.
108. E.N. Skountzos, F. von Wrochem, **V.G. Mavrantzas**,* "Structure and conformation of a crystalline P3HT film adsorbed on an alkanethiol self-assembled monolayer deposited on gold", *Macromol. Theory Simul.* **2020**, 2000010.
109. A.F. Katsarou, A.J. Tsamopoulos, D.G. Tsalikis,* **V.G. Mavrantzas**,* "Dynamic heterogeneity in ring-linear polymer blends", *Polymers* **2020**, *12*, 752.
110. S.D. Peroukidis, D.G. Tsalikis, M.G. Noro, I.P. Stott, **V.G. Mavrantzas**,* "Quantitative prediction of the size and shape of micelles formed in aqueous solutions of ionic surfactants: A combined approach based on coarse-grained MARTINI simulations followed by reverse-mapped all-atom molecular dynamics simulations", *J. Chem. Theory Comput.* **2020**, *16*, 3363-3372.
111. D.G. Tsalikis, T.S. Alexiou, P.V. Alatas, **V.G. Mavrantzas**,* "Conformation and diffusivity of ring and linear poly(ethylene oxide) in aqueous solution: Molecular topology dependent concentration effects and comparison with experimental data", *Macromol. Theory Simul.* **2020**, 2000016.
112. P.S. Stephanou,* I.Ch. Tsimouri, **V.G. Mavrantzas**, "Simple, accurate and user-friendly differential constitutive model for the rheology of entangled polymer melts and solutions from nonequilibrium thermodynamics", *Materials* **2020**, *13*, 2867.
113. T.S. Alexiou, P.V. Alatas, D.G. Tsalikis, **V.G. Mavrantzas**,* "Conformational and dynamic properties of short DNA minicircles in aqueous solution from atomistic molecular dynamics simulations", *Macromolecules* **2020**, 53, 5903−5918.
114. T.S. Alexiou, D.G. Mintis, **V.G. Mavrantzas**,* "Molecular dynamics simulation of the diffusion dynamics of linear DNA fragments in dilute solution with the PARMBSC1 force field and comparison with experimental data and theoretical models", *Macromolecules* **2020**, 53, 6135−6150.
115. D.G. Mintis, T.S. Alexiou, **V.G. Mavrantzas**,* "Effect of pH and Molecular Length on the Structure and Dynamics of Linear and Short-Chain Branched Poly(ethylene imine) in Dilute Solution: Scaling Laws from Detailed Molecular Dynamics Simulations", *J. Phys. Chem. B* **2020**, *124*, 6154−6169.
116. P.S. Stephanou,* I.Ch. Tsimouri, **V.G. Mavrantzas**, "Two-species models for the rheology of associative polymer solutions: Derivation from nonequilibrium thermodynamics", *J. Rheology* **2020**, *64*, 1003–1016.
117. F.D. Tsourtou, L. Peristeras,* R. Apostolov, **V.G. Mavrantzas**,* "Molecular Dynamics simulation of amorphous poly(3-hexyl thiophene)", *Macromolecules* **2020**, *53*, 7810−7824.
118. D.G. Mintis, **V.G. Mavrantzas**,* "Phase oundary and salt partitioning in coacervate complexes formed between poly(acrylic acid) and poly(N,N-dimethylaminoethyl methacrylate) from detailed atomistic simulations combined wibth free energy perturbation and thermodynamic integration calculations", *Macromolecules* **2020**, *53*, 7618−7634.
119. P.G. Mermigkis, **V.G. Mavrantzas**,* "Geometric analysis of clusters of free volume accessible to small penetrants and their connectivity in polymer nanocomposites containing carbon nanotubes", *Macromolecules* **2020**, *53*, 9563−9583.
120. **V.G. Mavrantzas**,* "Using Monte Carlo to simulate complex polymer systems: Recent

progress and outlook", *Frontiers in Physics* **2021**, *9*, 661367.

121. E.N. Skountzos, D.G. Tsalikis, P.S. Stephanou, **V.G. Mavrantzas**,* "Individual contributions of adsorbed and free chains to microscopic dynamics of unentangled poly(ethylene glycol) - silica nanocomposite melts and the important role of end groups: Theory and simulation", *Macromolecules* **2021**, *54*, 4470-4487.
122. S.D. Peroukidis, D.G. Mintis, I. Stott, **V.G. Mavrantzas**,* "Molecular simulation of the morphology and viscosity of aqueous micellar solutions of sodium lauryl ether sulfate (SLEnS)", *J. Physics: Materials* **2021**, *4*, 044001.
123. A. Weyman, **V.G. Mavrantzas**,* H.C. Öttinger, "Field-theoretic simulations beyond δ-interactions: Overcoming the inverse potential problem in auxiliary field models", *J. Chem. Phys.* **2021**, *155*, 024106.
124. E.N. Skountzos, K.S. Karadima, **V.G. Mavrantzas**,* "Structure and dynamics of highly attractive polymer nanocomposites in the semi-dilute regime: The role of interfacial domains and bridging chains", *Polymers* **2021**, *13*, 2749.
125. P.V. Alatas, **V.G. Mavrantzas**,* H.C. Öttinger, "Third-order perturbation expansion of the two-point correlation function of the dissipative quantum φ^4 theory", *Phys. Rev. D* **2021**, *104*, 076007.
126. A. Weyman, **V.G. Mavrantzas**,* H.C. Öttinger, "Direct calculation of the functional inverse of realistic interatomic potentials in field-theoretic simulations", *J. Chem. Phys.* **2022**, *156*, 224115.
127. S.D. Peroukidis, I.P. Stott, **V.G. Mavrantzas**,* "A coarse-grained model incorporating short- and long-range effective potentials for the fast simulation of micelle formation in solutions of ionic surfactants", *J. Phys. Chem. B* **2022***, 126*, 5555–5569 *(Special Doros N. Theodorou Festschrift Issue)*.
128. A. Weyman, **V.G. Mavrantzas**,* "Excluded-Volume Interactions in Field-Theoretic Simulations: Multiconvolutions and Model Equivalence", *J. Phys. Chem. B* **2022**, *126*, 10948−10954.
129. P.S. Stephanou,* P. Vafeas, **V.G. Mavrantzas**,* "Non-equilibrium thermodynamics modelling of the stress-strain relationship in soft two-phase elastic-viscoelastic materials", *J. Non Equilib. Thermodyn.* **2023**, *48*, 91–105.
130. T. Mermigkis, K.S. Karadima, S.N. Pandis, **V.G. Mavrantzas**, "Geometric Analysis of Free and Accessible Volume in Atmospheric Nanoparticles", *ACS Omega* **2023**, *8*, 33481−33492.
131. D.G. Tsalikis, **V.G. Mavrantzas**, S.E. Pratsinis,* "Dynamics of molecular collisions in air and its mean free path", *Physics of Fluids* **2023**, *35*, 097131.
132. **V.G. Mavrantzas**,* "Relativistic hydrodynamics from the single-generator bracket formalism of nonequilibrium thermodynamics", *J. Non-Equilib. Thermodyn.* **2024**, *49*, 89–112.
133. D.G. Tsalikis, **V.G. Mavrantzas**, S.E. Pratsinis,* "A new equation for the mean free path of air", *Aerosol Science and Technology* **2024**, *58*, 930–941.
134. P. Siachouli, K.S. Karadima, **V.G. Mavrantzas**,* S.N. Pandis,* "The effect of functional groups on the glass transition temperature of atmospheric organic compounds: A molecular dynamics study", *Soft Matter* **2024**, *20*, 4783-4794.
135. P. Siachouli, **V.G. Mavrantzas**,* S.N. Pandis,* "Predicting and parameterizing the glass transition temperature of atmospheric organic aerosol components via molecular dynamics simulations", *Soft Matter* **2025**, *21*, 3880-3889.
136. K.S. Karadima, D.G. Tsalikis, **V.G. Mavrantzas**,* S.E. Pratsinis,* "Aerosol Particle Diffusivity in the Free Molecule Regime", *J. Phys. Chem. A* **2025**, *129*, 5127−5136.
137. D.G. Mintis, M. Dompé, P.D. Kolokathis, J. van der Gucht, A. Afantitis, **V.G. Mavrantzas**,* "Effect of pH, Temperature, Molecular Weight and Salt Concentration on the Structure and Hydration of Short Poly(N,N-dimethylaminoethyl methacrylate) Chains in Dilute Aqueous Solutions: A Combined Experimental and Molecular Dynamics Study", *Polymers* **2025**, *17*, 2189.
138. P. Panagopoulos Papageorgiou, K.S. Karadima,* I. Papageorgiou, **V.G. Mavrantzas**,* "Structural properties and conformational dynamics of keratin-derived antimicrobial peptides from molecular dynamics simulations", *J. Chem. Information Modeling* **2025**, submitted.
139. M. D'Andria, M. Yin, **V.G. Mavrantzas**, Y. Chen, K. Suzuki, A.T. Güntner,* "Polymorph-Specific Electronic Transduction in WO3 during Molecular Sensing", *Advanced Materials* **2025**, submitted.

140. P. Siachouli, **V.G. Mavrantzas**,* S.N. Pandis,* "Predicting the self-diffusion coefficient of atmospheric organic aerosol components via molecular dynamics simulations", *Soft Matter* **2025**, in preparation.

CHAPTERS IN BOOKS

1. **V.G. Mavrantzas**, *Wall effects in polymer solutions*, Chapter in: A.N. Beris and B.J. Edwards, "Thermodynamics of Flowing Systems with Internal Microstructure", Oxford Univ. Press, New York, **1994**.
2. V.A. Harmandaris, **V.G. Mavrantzas**, *Molecular Dynamics Simulations of Polymers*, Chapter in: "Simulation Methods for Modeling Polymers", Edited by D.N. Theodorou and M.J. Kotelyanskii, Marcel Dekker, **2002.**
3. **V.G. Mavrantzas**, *Monte Carlo Simulation of Chain Molecules*, Chapter in: "Handbook of Materials Modeling. Volume I: Models and Methods", Edited by S. Yip, Springer, The Netherlands, pp. 1-15, **2005**.
4. N.Ch. Karayiannis, **V.G. Mavrantzas**, *Atomistic Monte Carlo methods for the atomistic simulation of polymers with a linear or non-linear molecular architecture*. In: "Multiscale modelling of polymer properties", edited by E. Perpète and M. Laso, Vol. 22 of the Computer-Aided Chemical Engineering book series, edited by R. Gani, Elsevier, **2006**.
5. N.Ch. Karayiannis, **V.G. Mavrantzas**, D. Mouratidis, E. Chiotelis, C.D. Kyparissides, *Atomistic Molecular dynamics simulation of short-chain branched polyethylene melts*. In: "Polymer Modeling at Multiple Time and Length Scales", edited by E. Perpète and M. Laso, Vol. 22 of the Computer-Aided Chemical Engineering book series, edited by R. Gani, Elsevier, **2006**.
6. V.A. Harmandaris, **V.G. Mavrantzas**, *Segmental dynamics in polyethylene melts through atomistic molecular dynamics simulations*. In: "Recent Research Topics and Developments in Chemical Physics: From Quantum Scale to Macroscale", edited by A.F. Terzis, Research Signpost, **2007.**
7. **V.G. Mavrantzas**, *Polymer melt viscoelasticity: What can we learn from molecular simulations*. In: "Rheology Reviews", British Society of Rheology, **2008**.
8. G. Tsolou, **V.G. Mavrantzas**, *Hierarchical modelling of polymeric systems at multiple time and length scales*. In: "Applications of Molecular Systems Engineering - Part I", edited by C.S. Adjiman and A. Galindo, Vol. 6 of the Process Systems Engineering book series, edited by E. N. Pistikopoulos, M. C. Georgiadis and V. Dua, Wiley-VCH, **2010**.
9. **V.G. Mavrantzas**, *Molecular Modelling*. In: "Encyclopedia for Life Support Sciences (EOLSS)", Chemical Engineering and Chemical Process Technology: 1. Fundamentals of Chemical Engineering, edited by R. Pohorecki, J. Bridgwater, M. Molzahn, and R. Gani, **2010**.
10. P. Ilg, **V.G. Mavrantzas**, H.C. Öttinger, *Multiscale Modeling and Coarse Graining of Polymer Dynamics: Simulations Guided by Statistical Beyond-Equilibrium Thermodynamics*. In: "Modeling and Simulations in Polymers", edited by P.D. Gujrati and A. L. Leonov, Wiley-VCH, **2011**.
11. E.N. Skountzos, **V.G. Mavrantzas**, *Molecular dynamics simulations of graphene-based polymer nanocomposites.* In: "Carbon-based Smart Materials", edited by C.A. Charitidis, E.P. Koumoulos and D.A. Dragatogiannis, De Gruyter, **2020**.

SPECIAL JOURNAL VOLUMES EDITED

1. **V.G. Mavrantzas**, A.N. Beris, Th. Tzavaras (Guest Editors), Special Volume on: *Non-equilibrium Thermodynamics and Complex Fluids*, Journal of Non-Newtonian fluid Mechanics (JNNFM), Volume 152, Issues 1-3, **2008**.
2. **V.G. Mavrantzas**, P.S. Stephanou (Guest Editors): *Theory and Simulations of Entangled Polymers*, Polymers, 17 published papers, **2018-2019**.
3. **V.G. Mavrantzas**, L.D. Peristears, C. Baig (Guest Editors): *Monte Carlo Simulation of Soft Matter Systems*, Frontiers in Phyics, Special Volume, project in progress, **2020**.
4. **V.G. Mavrantzas**, D.N. Theodorou (Guest Editors): *Coarse-Grained Models for Polymers*, Polymers, Special Volume, project in progress, **2021-2022**.

BOOKS Written

1. **V.G. Mavrantzas,** *Statistical Thermodynamics* (in Greek), book for the course on "Physical Chemistry", Studies in Natural Sciences, Hellenic Open University, Patras, **2001.**

2. D.N. Theodorou, **V.G. Mavrantzas,** *Multi-scale Modelling of Polymers*, Oxford Univ. Press, Oxford (UK), **2024** submitted. Book contains the following 10 chapters:
   Chapter 1: Models for polymer chains
   Chapter 2: From electronic structure calculations to classical force fields
   Chapter 3: Molecular mechanics
   Chapter 4: Molecular dynamics
   Chapter 5: Monte Carlo
   Chapter 6: Techniques for the analysis and simulation of infrequent events
   Chapter 7: Coarse-graining
   Chapter 8: Entanglement network-based simulations of deformation and flow
   Chapter 9: Dissipative particle dynamics
   Chapter 10: Beyond-equilibrium simulations based on principles of nonequilibriumtermodynamics

PUBLICATIONS IN CONFERENCE PROCEEDINGS

1. **V.G. Mavrantzas**, A.N. Beris, "Modeling and simulation of the dilute polymer solution flow behavior next to solid surfaces and interfaces", *Polymer Preprints*, Proceedings, *Symposium on Modeling and Computer Simulation,* National Meeting of the American Chemical Society, San Francisco, Vol. 33, pp. 615-619, April 5-10, **1992**.
2. **V.G. Mavrantzas**, D.N. Theodorou, "From chain chemical structure to polymer melt elasticity: The implementation of new Monte Carlo techniques", Proceedings*, 1st Panhellenic Chemical Engineers' Conference*, Patras, Greece, May 29-31, **1997**.
3. V.A. Harmandaris, **V.G. Mavrantzas**, D.N. Theodorou, "From chemical structure to polymer processing: Atomistic simulation of the viscoelasticity of linear polyethylene melts", Proceedings*, 4th Panhellenic Conference on Polymers*, Patras, Greece, November 20-22, **1997**.
4. M. Apostolakis, J. Hatzinicolaou, **V.G. Mavrantzas**, "Stress-induced polymer migration effects in the Taylor-Couette device: Numerical calculations with spectral elements", Proceedings, *2nd Panhellenic Chemical Engineers' Conference*, Salonica, Greece, May 27-29, **1999**.
5. E. Zervopoulou, **V.G. Mavrantzas**, D.N. Theodorou, "Atomistic simulation of the solubility of small alkanes in long polyethylene melts", Proceedings*, 2nd Panhellenic Chemical Engineers' Conference*, Salonica, Greece, May 27-29, **1999**.
6. V.A. Harmandaris, V.G. **Mavrantzas**, D.N. Theodorou, "Atomistic simulation of the stress relaxation experiment after cessation of steady-state uniaxial elongation", Proceedings, *2nd Panhellenic Chemical Engineers' Conference*, Salonica, Greece, May 27-29, **1999**.
7. V.A. Harmandaris, **V.G. Mavrantzas**, D.N. Theodorou, "Atomistic Modeling of Viscoelastic Properties: Simulation of stress relaxation upon cessation of steady state elongational flow", Proceedings, *International George Papatheodorou Symposium*, Patras, Greece, September 16-18, **1999.**
8. V.A. Harmandaris, **V.G. Mavrantzas**, D.N. Theodorou, "Prediction of the linear viscoelastic properties of long-chain polyethylene melts from detailed atomistic simulations on uniaxially stretched melt configurations", Proceedings, *XIII International Congress on Rheology*, pp. 2.76-2.78, Cambridge, UK, August 20-25, **2000**.
9. **V.G. Mavrantzas**, A.N. Beris, "Polymer depletion phenomena near a solid surface: Modeling the effect of a shear flow", Proceedings, *XIII International Congress on Rheology*, pp. 2.79-2.81, Cambridge, UK, August 20-25, **2000.**
10. M. Apostolakis, **V.G. Mavrantzas**, "Polymer diffusion in inhomogeneous flow fields: Pseudospectral calculations in the Taylor-Couette geometry", Les Cahiers de Rhéologie, Volume XVII, Numéro 1, 181-189, **2000**.
11. 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", Proceedings, *3rd Panhellenic Chemical Engineers' Conference*, Athens, Greece, May 31-June 02, **2001**.
12. 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", Proceedings, *3rd Panhellenic Chemical Engineers' Conference*, Athens, Greece, May 31-June 02, **2001**.
13. M. Apostolakis, **V.G. Mavrantzas**, A.N. Beris, "Polymer diffusion in the Taylor-Couette

geometry: Calculation of the time-dependent basic flow with pseudo-spectral elements", Proceedings, *3rd Panhellenic Chemical Engineers' Conference*, Athens, Greece, May 31-June 02, **2001.**

14. K.Ch. Daoulas, A.F. Terzis, **V.G. Mavrantzas**, "Melts of macromolecules grafted on a hard surface or graphite: Detailed atomistic simulation of their interfacial structure", Proceedings, *4th GRACM Congress on Computational Mechanics*, Patras, Greece, June 27-29, **2002**.
15. **V.G. Mavrantzas**, V.A. Harmandaris, D.N. Theodorou, "Hierarchical Modeling of the viscoelasticity of linear polymer melts", Proceedings, *4th GRACM Congress on Computational Mechanics*, Patras, Greece, June 27-29, **2002**.
16. V.A. Harmandaris, **V.G. Mavrantzas**, D.N. Theodorou, "Prediction of the viscoelastic properties of polymer from detailed molecular dynamics simulations and comparison against rheological measurements", Proceedings, *3rd Chemical Engineering Conference for Collaborative Research in Eastern Mediterranean (EMCC-3)*, Thessaloniki, Greece, May 13-15, **2003.**
17. K. Foteinopoulou, **V.G. Mavrantzas**, J. Tsamopoulos, "Numerical calculation of bubble growth in Newtonian and viscoleastic filaments undergoing stretching", Proceedings, pp. 805-808, *4th Panhellenic Chemical Engineers' Conference*, Patras, Greece, May 29-31, **2003**.
18. K. Daoulas, A.F. Terzis, **V.G. Mavrantzas**, "A novel method for precisely controlling the chain length distribution in atomistic simulations of inhomogeneous and/or anisotropic polymer systems with chain connectivity-altering Monte Carlo algorithms", Proceedings, pp. 501-504, *4th Panhellenic Chemical Engineers' Conference*, Patras, Greece, May 29-31, **2003**.
19. G. Tsolou, **V.G. Mavrantzas**, D.N. Theodorou, "Atomistic molecular dynamics simulations of cis-1,4 polybutadiene melts", Proceedings, pp. 37-40, *4th Panhellenic Chemical Engineers' Conference*, Patras, Greece, May 29-31, **2003.**
20. K.Ch. Daoulas, **V.G. Mavrantzas**, "Atomistic Monte Carlo simulation studies of polymer melts grafted on solid substrates", Proceedings, *International Conference on Computational Methods in Sciences and Engineering (ICCMSE 2003)*, Kastoria, Greece, September 12-16, **2003**.
21. K.Ch. Daoulas, **V.G. Mavrantzas**, "Detailed atomistic simulation of tethered polymer melts", *Advances in Science and Technology: Computational Modeling and Simulation of Materials III, Part A*, Edited by: P. Vincenzini and A. Lami), Vol. 42, pp. 605-612, **2004.**
22. V.A. Harmandaris, K.Ch. Daoulas, **V.G. Mavrantzas**, "Atomistic simulation of the structure and dynamics of the polyethylene/graphite interface", *Advances in Science and Technology: Computational Modeling and Simulation of Materials III, Part A*, Edited by: P. Vincenzini and A. Lami), Vol. 42, pp. 557-564, **2004.**
23. N.Ch. Karayiannis, **V.G. Mavrantzas**, "Detailed atomistic simulation of long chain branched polyethylene melts", *Advances in Science and Technology: Computational Modeling and Simulation of Materials III, Part A*, Edited by: P. Vincenzini and A. Lami), Vol. 42, pp. 397-404, **2004.**
24. **V.G. Mavrantzas**, D.N. Theodorou, H.C. Öttinger, "Thermodynamically founded hierarchical methodologies for the simulation of polymer melts beyond equilibrium: detailed atomistic simulation of polymer melt viscoelasticity", *Advances in Science and Technology: Modeling and Simulating materials nanoworld*, Edited by: P. Vincenzini and F. Zerbetto), Vol. 44, pp. 301-307, **2004.**
25. **V.G. Mavrantzas**, D.N. Theodorou, H.C. Öttinger, "Thermodynamically founded atomistic Monte Carlo for the simulation of polymer melt viscoelasticity", Proceedings, *XIVth International Congress on Rheology,* pp. CR04-1 - CR04-3, Seoul, Korea, August 22-27, **2004.**
26. N.Ch. Karayiannis, **V.G. Mavrantzas**, "Detailed atomistic simulation of the conformational and dynamic properties of H-shaped polyethylene melts", Proceedings, *XIVth International Congress on Rheology,* pp. MS11-1 – MS11-3, Seoul, Korea, August 22-27, **2004.**
27. K. Foteinopoulou, **V.G. Mavrantzas**, J. Tsamopoulos, "Numerical Simulation of cavitation dynamics during the extensional flow of a polymeric filament", Proceedings, *FLOW 2004 Meeting*, Athens, Greece, November, **2004**.
28. O. Alexiadis, K.Ch. Daoulas, **V.G. Mavrantzas**, "Atomistic Monte Carlo simulation of alkanethiol based self-assembled monolayers on the Au(111) surface", Proceedings, *5th Panhellenic Chemical Engineers Conference*, Thessaloniki, Greece, May 26-28, **2005**.
29. G. Tsolou, V.A. Harmandaris, **V.G. Mavrantzas**, "Atomistic molecular dynamics simulation of

pressure and temperature effects on *cis*-1,4 polybutadiene and polyethyene", Proceedings, *5th Panhellenic Chemical Engineers Conference*, Thessaloniki, Greece, May 26-28, **2005.**

30. N. Ch. Karayiannis, **V.G. Mavrantzas**, "Calculation of branch point friction and chain reptation time of H-shaped polyethylene melts from long atomistic molecular dynamics simulations", Proceedings, *5th Panhellenic Chemical Engineers Conference*, Thessaloniki, Greece, May 26-28, **2005**.
31. K. Foteinopoulou, **V.G. Mavrantzas**, J. Tsamopoulos, "Numerical simulation of multi-bubble growth in filaments undergoing stretching", Proceedings, *5th Panhellenic Chemical Engineers Conference*, Thessaloniki, Greece, May 26-28, **2005**.
32. 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)", Proceedings, *5th Panhellenic Chemical Engineers Conference*, Thessaloniki, Greece, May 26-28, **2005**.
33. K. Foteinopoulou, **V.G. Mavrantzas**, J. Tsamopoulos, "Numerical simulation of multi-bubble growth in filaments undergoing stretching", Proceedings, *5th GRACM International Congress on Computational Mechanics*, Limassol, Cyprus, June 29-July 1, **2005.**
34. V. Soni, J. Abildskov, G. Jonsson, R. Gani, N. Karayiannis, **V.G. Mavrantzas**, "Structural design of polymers for membrane-based separation processes using reverse simulation approach", *16th European Symposium on Computer Aided Process Engineering (Escape-16)* and *9th International Symposium on Process Systems Engineering (PSE 2006), Book Series: Computer-Aided Chemical Engineering,* Vol. 21, pp. 689-694, Garmisch-Partenkirchen, Germany, July 09-13, **2006**.
35. P.S. Stephanou, C. Baig, **V.G. Mavrantzas**, "Generalizing the Giesekus model so that it can account for chain finite-extensibility effects and analysis of its predictions for polymer melts in viscometric flows", Proceedings, *6thPanhellenic Chemical Engineers Conference*, Athens, Greece, May 31-June 2, **2007**.
36. K.C. Satyanarayana, J. Abildskov, R. Gani, G. Tsolou, **V.G. Mavrantzas**, "Multiscale modelling for computer aided polymer design", Proceedings, *10th International Symposium on Process Systems Engineering (PSE 2009), Book Series: Computer-Aided Chemical Engineering*, Vol. 27, pp. 213-218, Salvador, Brazil, August 16-20, **2009**.
37. C. Baig, P.S. Stephanou, **V.G. Mavrantzas**, "Multiscale simulation of polymer melt viscoelasticity guided from nonequilibrium statistical thermodynamics: Atomistic nonequilibrium thermodynamics coupled with Monte Carlo in an expanded statistical ensemble", Proceedings, *7th Panhellenic Chemical Engineers Conference*, Patras, Greece, June 3-5, **2009**.
38. P.S. Stephanou, C. Baig, G. Tsolou, **V.G. Mavrantzas**, M. Kröger, "Quantifying chain reptation in entangled polymer melts: Topological and dynamical mapping of atomistic simulation results onto the tube model", Proceedings, *7th Panhellenic Chemical Engineers Conference*, Patras, Greece, June 3-5, **2009**.
39. G. Tsolou, **V.G. Mavrantzas**, "Study of the unique dynamic, barrier and glass tarnsistio properties of polyisobutylene through detailed molecular dynamics simulations", Proceedings, *7th Panhellenic Chemical Engineers Conference*, Patras, Greece, June 3-5, **2009.**
40. C. Baig, O. Alexiadis, **V.G. Mavrantzas**, "Advanced Monte Carlo moves for the atomistic simulation of polymer melts with a variety of molecular architectures", Proceedings, *4th International Conference from Scientific Computing to Computational Engineering (4th IC-SCCE)*, Athens, Greece, July 7-10, **2010**.
41. P.S. Stephanou, C. Baig, G. Tsolou, **V.G. Mavrantzas**, "Mapping atomistic simulation results for the dynamics of entangled polymer melts onto the tube model of the reptation theory", Proceedings, *4th International Conference from Scientific Computing to Computational Engineering (4th IC-SCCE)*, Athens, Greece, July 7-10, **2010**.
42. G.N. Nomikos, D.I. Kondarides, **V.G. Mavrantzas**, X.E. Verykios, "Photocatalytic reactor design for energy and environmental applications", Proceedings, *8th Panhellenic Chemical Engineers Conference*, Thessaloniki, Greece, May 26-28, **2011**.
43. G.N. Nomikos, D.I. Kondarides, **V.G. Mavrantzas**, X.E. Verykios, "Photocatalytic reactor design for energy and environmental applications", Proceedings, *2011 International Conference on H_2 production (ICH2P-2011)*, Thessaloniki, Greece, June 19-22, **2011**.
44. P.S. Stephanou, C. Baig, **V.G. Mavrantzas**, "Generalized viscoelastic model for polymer melts

guided by principles of non-equilibrium thermodynamics: single- and multi-mode formulations", Proceedings, *7th GRACM International Congress on Computational Mechanics (7th GRACM)*, Athens, Greece, June 30- July 2, **2011**.

45. A. Anastasiou, C. Baig, **V.G. Mavrantzas**, "Non-equilibrium molecular dynamics simulation of the stretching behavior of adhesive polymers", Proceedings, *7th GRACM International Congress on Computational Mechanics (7th GRACM)*, Athens, Greece, June 30- July 2, **2011**.

46. D. Tsalikis, C. Baig, **V.G. Mavrantzas**, E. Amanatidis, D. Mataras, "Hierarchical simulation of microcrystalline PECVD silicon film growth and structure", Proceedings, *13th International Conference on Plasma Surface Engineering (PSE 2012),* Garmisch-Partenkirchen, Germany, September 10 - 14, **2012**.

47. D. Tsalikis, C. Baig, **V.G. Mavrantzas**, E. Amanatidis, D. Mataras, "Hierarchical simulation of microcrystalline silicon thin films growth and structure", Proceedings, *27th European Photovoltaic Solar Energy Conference and Exhibition (EU PSVEC 2012),* Messe Frankfurt, Germany, September 25-28, **2012**.

48. 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**.

49. 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**.

50. E. Skountzos, A. Anastassiou, S. Sabethai, **V.G. Mavrantzas**, D.N. Theodorou, "Polymer-graphene nanocomposites: atomistic modeling and simulation of their mechanical properties", Proceedings, *9th Panhellenic Chemical Engineers Conference*, Athens, Greece, May 23-25, **2013**.

51. 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, *9th Panhellenic Chemical Engineers Conference*, Athens, Greece, May 23-25, **2013**.

52. 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", Proceedings, *9th Panhellenic Chemical Engineers Conference*, Athens, Greece, May 23-25, **2013**.

53. 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**.

54. K.S. Karadima, **V.G. Mavrantzas**, S.N. Pandis, "A molecular dynamics simulation study of atmospheric nanoparticles", *10th Panhellenic Chemical Engineers Conference*, Patras, Greece, June 4-6, **2015**.

55. 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**.

56. 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**.

57. 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**.

58. 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**.

59. 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**.

60. 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**.

61. 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**.

62. 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**.
63. 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**.
64. 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**.
65. 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**.
66. 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**.
67. 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**.
68. 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.**
69. 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.**
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.**
72. P.V. Alatas, D.G. Tsalikis, **V.G. Mavrantzas**, "Comparison of the conformational and dynamic properties between ring and linear polyethylene oxide melts in the crossover region from unentangled to entangled through molecular dynamics simulations", *11th Panhellenic Chemical Engineers Conference*, Salonica, Greece, May 25-27, **2017.**
73. 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.**
74. 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.**
75. 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.**
76. 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.**
77. A. Spyrogianni, K.S. Karadima, E. Goudeli, **V.G. Mavrantzas**, S.E. Pratsinis, "Brownian dynamics simulation of the settling rate of fractal-like nanoparticle agglomerates", *11th Panhellenic*

Chemical Engineers Conference, Salonica, Greece, May 25-27, **2017.**

78. K.S. Karadima, **V.G. Mavrantzas**, S.N. Pandis, "Diffusion coefficients and viscosities of organic aerosol components through equilibrium and non-equilibrium molecular dynamics simulations", https://doi.org/10.5194/egusphere-egu21-4141, *EGU General Assembly (EGU21-4141)*, April 19-30, **2021**.
79. P. Siachouli, K.S. Karadima, **V.G. Mavratzas**, S.N. Pandis, "On the glass transition temperature of organic compounds via molecular dynamics simulations", https://doi.org/10.5194/egusphere-egu22-6382, *EGU General Assembly (EGU22)*, Vienna, Austria, May 23-27, **2022**.
80. P.G. Mermigkis, K.S. Karadima, **V.G. Mavratzas**, S.N. Pandis, "On the Phase State of Aerosol Nanoparticles from a detailed Geometric Analysis of their Free Volume Accessible to Small Penetrants", https://doi.org/10.5194/egusphere-egu22-13250, *EGU General Assembly (EGU22)*, Vienna, Austria, May 23-27, **2022**.
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**.
82. 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**.
83. 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**.
84. T. Mermigkis, K.S. Karadima, **V.G. Mavrantzas**, 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**.
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**.
86. 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**.

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**.
8. **V.G. Mavrantzas**, A.N. Beris, "Rheology of dilute polymer solutions in the adjacency of a solid surface", *AIChE Annual Meeting*, Saint Lewis, November 7-11, **1993**.
9. **V.G. Mavrantzas**, A.N. Beris, "Polymer migration in simple viscometric flows", *AIChE Annual Meeting*, Saint Lewis, November 7-11, **1993**.

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**.
13. **V.G. Mavrantzas**, V.A. Harmandaris, D.N. Theodorou, "Atomistic simulation of the viscoelasticity of linear polyethylene melts", *1st Hellenic Society of Rheology Meeting*, Heraklion, Greece, August 29-September 2, **1998**.
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**.
17. V.A. Harmandaris, **V.G. Mavrantzas**, D.N. Theodorou, "Atomistic Modeling of Viscoelasticity: Simulation of stress relaxation upon cessation of steady-state elongational flow", *Summer School in Polymer Science and Technology*, Psathopirgos, Patras, Greece, September 5-9, **1999**.
18. **V.G. Mavrantzas**, A.N. Beris, "A hierarchical, self-consistent model for the study of surface effects on the structure and rheology of polymer solutons. I) General formulation with application to the flow past a wall, II) Application to an adsorbing surface", Proceedings, *Interfaces and Colloidal Systems*, Aghia Pelaghia, Heraklion Crete, Greece, September 18-23, **1999**.
19. **V.G. Mavrantzas**, H.C. Öttinger, "GENERIC: A guide for the design of atomistic Monte Carlo simulations for nonequilibrium systems", *Nonequilibrium Thermodynamics and Complex Fluids*, Oxford, UK, August 14-18, **2000**.
20. V.A. Harmandaris, **V.G. Mavrantzas**, D.N. Theodorou, "Prediction of the linear viscoelastic 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.**
22. K.Ch. Daoulas, **V.G. Mavrantzas**, D. Photinos, "Grafted Polymer Melts: Detailed Atomistic Simulation of their Interfacial Structure", *3rd COST P1 Workshop on Soft Condensed Matter*, Patras, September 22-23, **2000**.
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.**
26. **V.G. Mavrantzas**, E. Zervopoulou, M. Doxastakis, D.N. Theodorou, "Prediction of Physical Properties of Polymer Melts", *AIChE Annual Meeting*, Los Angeles, November 13-17, **2000.**
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**.
30. M. Apostolakis, **V.G. Mavrantzas**, A.N. Beris, "Polymer diffusion in the Taylor-Couette geometry: Calculation of the time-dependent basic flow with pseudo-spectral elements", *3rd Panhellenic Chemical Engineers' Conference*, Athens, Greece, May 31-June 02, **2001.**
31. M. Apostolakis, **V.G. Mavrantzas**, A.N. Beris, "Stress-induced migration effects on the viscoelastic Taylor-Couette flow", *3rd International Meeting of the Hellenic Society of Rheology*, Patras, Greece, June 10-14, **2001.**
32. V.A. Harmandaris, **V.G. Mavrantzas**, D.N. Theodorou, "Prediction of the rheological properties of long polyethylene melts via atomistic molecular dynamics simulations", *3rd International Meeting of the Hellenic Society of Rheology*, Patras, Greece, June 10-14, **2001.**
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.**
35. Daoulas, K.; Terzis, A.F.; **Mavrantzas, V.G.,** "Detailed end-bridging Monte Carlo simulations of polymer melts grafted on a solid substrate", Proceedings*, 5th Hellenic Polymer Society Symposium (ELEP 2001)*, Heraklion, Crete, December 15-17, **2001**.
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**.
37. **V.G. Mavrantzas**, V.A. Harmandaris, D.N. Theodorou, "Atomistic Monte Carlo simulations of the viscoelastic properties of polymer melts", *4th GRACM Congress on Computational Mechanics*, Patras, Greece, June 27-29, **2002**.
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**.
39. **V.G. Mavrantzas**, A.N. Beris, "Modeling interfacial effects on the conformation and rheology of polymer solutions through a hierarchical, continuum model", *Chain Molecules at Interfaces, A Symposium to the memory of Jan Scheutjens*, Wageningen University, The Netherlands, August 25-28, **2002.**
40. K.Ch. Daoulas, **V.G. Mavrantzas**, "Detailed atomistic Monte Carlo simulation of grafted polymer melts: Thermodynamic, conformational and structural properties", *Chain Molecules at Interfaces, A Symposium to the memory of Jan Scheutjens*, Wageningen University, The Netherlands, August 25-28, **2002**.
41. N.Ch. Karayiannis, **V.G. Mavrantzas**, "A novel Monte Carlo scheme for the detailed simulation of nonlinar H-shaped model polyethylene melts", *XVIII Panhellenic Conference on Solid State Physics-Materials Science,* Heraklion, Crete, September 15-18, **2002**.
42. K.Ch. Daoulas, **V.G. Mavrantzas**, "Detailed atomistic Monte Carlo simulation of grafted polymer melts", *Euresco,* Spain, September 14-19, **2002**.
43. V.A. Harmandaris, **V.G. Mavrantzas**, D.N. Theodorou, "Prediction of the viscoelastic properties of polymer from detailed molecular dynamics simulations and comparison against rheological measurements", *3rd Chemical Engineering Conference for Collaborative Research in Eastern Mediterranean (EMCC-3)*, Thessaloniki, Greece, May 13-15, **2003.**
44. K. Foteinopoulou, **V.G. Mavrantzas**, J. Tsamopoulos, "Numerical calculation of bubble growth in Newtonian and viscoleastic filaments undergoing stretching", *4th Panhellenic Chemical Engineers' Conference*, Patras, Greece, May 29-31, **2003**.
45. K.Ch. Daoulas, A.F. Terzis, **V.G. Mavrantzas**, "A novel method for precisely controlling the chain length distribution in atomistic simulations of inhomogeneous and/or anisotropic polymer systems with chain connectivity-altering Monte Carlo algorithms", *4th Panhellenic Chemical Engineers'*

Conference, Patras, Greece, May 29-31, **2003**.

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.**
47. K. Foteinopoulou, **V.G. Mavrantzas**, J. Tsamopoulos, "Numerical simulation of bubble growth during filament stretching of pressure-sensitive adhesive materials", *XIIIth International Workshop on Numerical Methods for non-Newtonian flows",* Lausanne, Switzerland, June 4-7, **2003**.
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**.
49. **V.G. Mavrantzas**, "Modeling interfacial effects on the conformation and rheology of polymer solutions through a hierarchical, continuum model", *3rd International Workshop on Non-Equilibrium Thermodynamics and Complex Fluids (3rd IWNET)*, Princeton, USA, August 14-17, **2003**.
50. K. Foteinopoulou, **V.G. Mavrantzas**, J. Tsamopoulos, "Numerical Simulation of bubble growth during filament stretching", *The 5th Euromech Fluid Mechanics Conference*, Toulouse, France, August 24-28, **2003**.
51. K.Ch. Daoulas, **V.G. Mavrantzas**, "Atomistic Monte Carlo simulation studies of polymer melts grafted on solid substrates", *International Conference on Computational Methods in Sciences and Engineering (ICCMSE 2003)*, Kastoria, Greece, September 12-16, **2003**.
52. V.A. Harmandaris, **V.G. Mavrantzas**, D.N. Theodorou, "Molecular Dynamics simulation of the viscoelastic properties of linear polymer melts", *Polymer Processing Society (PPS)*, Athens, Greece, September 14-17, **2003**.
53. N.Ch. Karayiannis, **V.G. Mavrantzas,** D.N. Theodorou, "Study of the segmental dynamics and barrier properties of amorphous PET [poly(ethylene terephthalate)] and PEI [poly(ethylene isophthalate)] through atomistic simulations", *AIChE Annual Meeting*, San Francisco, USA, November 16-21, **2003.**
54. N.Ch. Karayiannis, **V.G. Mavrantzas**, "An advanced Monte Carlo algorithm for the fast equilibration of atomistic models of H-shaped polyethylene melts", *AIChE Annual Meeting*, San Francisco, USA, November 16-21, **2003.**
55. V.A. Harmandaris, **V.G. Mavrantzas**, D.N. Theodorou, "Atomistic molecular dynamics simulation of n-alkane self-diffusion in melts and binary blends", *AIChE Annual Meeting*, San Francisco, USA, November 16-21, **2003.**
56. V.A. Harmandaris, **V.G. Mavrantzas**, D.N. Theodorou, "Atomistic molecular dynamics simulation of the viscoelastic properties of long-chain polyethylene melts: Crossover from Rouse to reptation regime", *AIChE Annual Meeting*, San Francisco, USA, November 16-21, **2003.**
57. K.Ch. Daoulas, **V.G. Mavrantzas**, "Detailed atomistic Monte Carlo simulation of long-chain end-grafted polymer melts", *AIChE Annual Meeting*, San Francisco, USA, November 16-21, **2003.**
58. **V.G. Mavrantzas**, H.C. Öttinger, "GENERIC Monte Carlo: A thermodynamically founded Monte Carlo for the hierarchical simulation of complex systems under steady-state flow conditions", *AIChE Annual Meeting*, San Francisco, USA, November 16-21, **2003.**
59. K. Foteinopoulou, **V.G. Mavrantzas**, J. Tsamopoulos, "Bubble growth during filament stretching of pressure sensitive adhesive materials", *AIChE Annual Meeting*, San Francisco, USA, November 16-21, **2003.**
60. K.Ch. Daoulas, **V.G. Mavrantzas**, "An atomistic simulation approach to the thermodynamics and structural properties of grafted polymer melts", *3rd International Conference on Computational Modeling and Simulation of Materials: From the Atomistic to the Engineering Scales*, Acireale (Catania), Italy, May 30 – June 4, **2004.**
61. V.A. Harmandaris, K.Ch. Daoulas, **V.G. Mavrantzas**, "Atomistic simulation of the structure and dynamics of the polyethylene/graphite interface", *3rd International Conference on Computational Modeling and Simulation of Materials: From the Atomistic to the Engineering Scales*, Acireale (Catania), Italy, May 30 – June 4, **2004.**
62. N.Ch. Karayiannis, **V.G. Mavrantzas**, "Detailed atomistic simulation of long-cahin branched polyethylene melts", *3rd International Conference on Computational Modeling and Simulation of*

Materials: From the Atomistic to the Engineering Scales, Acireale (Catania), Italy, May 30 – June 4, **2004.**

63. **V.G. Mavrantzas**, D.N. Theodorou, H.C. Öttinger, "Thermodynamically founded hierarchical methodologies for the simulation of polymer melts beyond equilibrium: detailed atomistic simulation of polymer melt viscoelasticity", *3rd International Conference on Computational Modeling and Simulation of Materials: From the Atomistic to the Engineering Scales*, Acireale (Catania), Italy, May 30 – June 4, **2004.**
64. K. Foteinopoulou, **V.G. Mavrantzas**, J. Tsamopoulos, "Numerical simulation of bubble growth during filament stretching of Newtonian and viscoelastic fluids", *4th International Meeting of the Hellenic Society of Rheology,* Athens, Greece, June 27-29, **2004.**
65. G. Tsolou, **V.G. Mavrantzas**, "Atomistic simulation of the dynamics of cis-1,4 polyboutadiene and its dependence on pressure and temperature", *4th International Meeting of the Hellenic Society of Rheology,* Athens, Greece, June 27-29, **2004.**
66. N.Ch. Karayiannis, **V.G. Mavrantzas**, "Branch point friction and its role in the dynamics of H-shaped polyethylene melts as probed by long molecular dynamics simulations", *4th International Meeting of the Hellenic Society of Rheology,* Athens, Greece, June 27-29, **2004.**
67. N.Ch. Karayiannis, **V.G. Mavrantzas**, "Detailed atomistic simulation of the conformational and dynamic properties of H-shaped polyethylene melts", *XIVth International Congress on Rheology,* Seoul, Korea, August 22-27, **2004.**
68. **V.G. Mavrantzas**, D.N. Theodorou, H.C. Öttinger, "Thermodynamically founded atomistic Monte Carlo for the simulation of polymer melt viscoelasticity", *XIVth International Congress on Rheology,* Seoul, Korea, August 22-27, **2004.**
69. N.Ch. Karayiannis, **V.G. Mavrantzas**, "Detailed atomistic simulation of the conformational and dynamic properties of H-shaped polyethylene melts", *XIVth International Congress on Rheology,* Seoul, Korea, August 22-27, **2004.**
70. K. Foteinopoulou, **V.G. Mavrantzas**, J. Tsamopoulos, "Numerical Simulation of cavitation dynamics in extensional flows of polymeric filaments", *FLOW 2004 Meeting*, Athens, Greece, November **2004**.
71. N.Ch. Karayiannis, **V.G. Mavrantzas**, "Role of branch point friction in the relaxation of H-polymers from detailed, 3μs-long, atomistic molecular dynamics simulations", *76th Annual Meeting of the Society of Rheology*, Lubock, USA, February 13-17, **2005.**
72. K. Foteinopoulou, **V.G. Mavrantzas**, J. Tsamopoulos, "Numerical calculation of the deformation of multiple bubbles in a filament undergoing stretching", *2nd Annual European Rheology Conference (AERC-2005),* Grenoble, France, April 21-23, **2005.**
73. O. Alexiadis, K.Ch. Daoulas, **V.G. Mavrantzas**, "Atomistic Monte Carlo simulation of alkanethiol based self-assembled monolayers on the Au(1,1,1) surface", *5th Panhellenic Chemical Engineers Conference*, Thessaloniki, Greece, May 26-28, **2005**.
74. N.Ch. Karayiannis, **V.G. Mavrantzas**, "Calculation of branch point friction and chain reptation time of H-shaped polyethylene melts from long atomistic molecular dynamics simulations", *5th Panhellenic Chemical Engineers Conference*, Thessaloniki, Greece, May 26-28, **2005**.
75. G. Tsolou, **V.G. Mavrantzas**, "Atomistic molecular dynamics simulation of pressure and temperature effects on cis-1,4 polybutadiene and polyethyene", *5th Panhellenic Chemical Engineers Conference*, Thessaloniki, Greece, May 26-28, **2005**.
76. V.A. Harmandaris, **V.G. Mavrantzas**, "Chain diffusion and mobility in thin films of polyethylene melts adsorbed on graphite through atomistic simulations", *European Polymer Congress*, Moscow, Russia, June 27-July 1, **2005.**
77. K. Foteinopoulou, **V.G. Mavrantzas**, J. Tsamopoulos, "Numerical simulation of multi-bubble growth in filaments undergoing stretching", *5th GRACM International Congress on Computational Mechanics,* Limassol, Cyprus, June 29-July 1, **2005.**
78. N.Ch. Karayiannis, **V.G. Mavrantzas**, "Calculation of branch point friction and chain reptation time of H-shaped polyethylene melts from long atomistic molecular dynamics simulations", CECAM Meeting on: *Modeling and Simulation of Entangled polymeric liquids*, Lyon, France, July 18-21, **2005.**
79. **V.G. Mavrantzas**, K. Foteinopoulou, J. Tsamopoulos, "On the deformation and translation of multiple bubbles in a viscoelastic filament undergoing stretching", SOR 77th Annual Meeting,

Vancouver, British Columbia, Canada, October 16-20, **2005**.

80. V. Soni, J. Abildskov, G. Jonsson, R. Gani, N. Karayiannis, **V.G. Mavrantzas**, "*Model based design of structured polymers using the reverse design approach*", *AIChE Annual Meeting*, San Francisco, USA, November 16-21, **2005.**
81. T. Ionescu, B.J. Edwards, V.G. Mavrantzas, *"*Atomistic simulation of energetic and entropic elasticity in short-chain polyethylenes*" AIChE Annual Meeting*, Cincinnati, USA, Oct. 30-Nov. 4, **2005.**
82. N.Ch. Karayiannis, **V.G. Mavrantzas**, "Hierarchical modeling 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", *231st ACS National Meeting*, Atlanta, USA, March 26-30, **2006**.
83. G. Tsolou, **V.G. Mavrantzas**, "Atomistic molecular dynamics simulation of the temperature and pressure dependence of local and terminal relaxation in amorphous polyethylene and *cis*-1,4 polybutadiene", *231st ACS National Meeting*, Atlanta, USA, March 26-30, **2006**.
84. **V.G. Mavrantzas**, A.N. Beris, "Continuum formulation of the Scheutjens-Fleer lattice statistical theory for homopolymer adsorption from solution", *231st ACS National Meeting*, Atlanta, USA, March 26-30, **2006**.
85. G. Tsolou, **V.G. Mavrantzas**, "Atomistic molecular dynamics simulation of the temperature and pressure dependence of local and terminal relaxation in *cis*-1,4 polybutadiene", *3rd Annual European Rheology Conference (AERC 2006)*, Hersonissos, Crete, Greece, April 27- 29, **2006**.
86. K. Foteinopoulou, N.Ch. Karayiannis, **V.G. Mavrantzas**, M. Kröger, "Topological analysis of polyethylene melts: Results from a hierarchical modeling approach combining atomistic Monte Carlo and long molecular dynamics simulations followed by a direct analysis of entanglements (poster)", *3rd Annual European Rheology Conference (AERC 2006)*, Hersonissos, Crete, Greece, April 27- 29, **2006**.
87. T. Ionescu, B.J. Edwards, D.J. Keffer, **V.G. Mavrantzas**, "Thermodynamics of non-isothermal polymer melts: Experiment, theory and simulation", *4th International Workshop on Non-Equilibrium Thermodynamics and Complex Fluids (4th IWNET)*, Rhodes, Greece, September 3-7, **2006.**
88. N.Ch. Karayiannis, **V.G. Mavrantzas**, "Atomistic simulation of polymers with a non-linear molecular architecture: Calculation of branch point friction and chain reptation time of an H-shaped polyethylene melt (poster)", *4th International Workshop on Non-Equilibrium Thermodynamics and Complex Fluids (4th IWNET)*, Rhodes, Greece, September 3-7, **2006.**
89. K. Foteinopoulou, N.Ch. Karayiannis, **V.G. Mavrantzas**, M. Kröger, "Primitive path identification and entanglement statistics in polymer melts: results from a direct topological analysis on atomistically detailed polyethylene models", *4th International Workshop on Non-Equilibrium Thermodynamics and Complex Fluids (4th IWNET)*, Rhodes, Greece, September 3-7, **2006.**
90. V. Dimitriadis, N.Ch. Karayiannis, **V.G. Mavrantzas**, E. Chiotellis, D. Mouratides, C.D. Kiparissides, "Structure and dynamics of polyethylene melts bearing short chain branches frequently spaced along their backbone as revealed from atomistic simulations (poster)", *4th International Workshop on Non-Equilibrium Thermodynamics and Complex Fluids (4th IWNET)*, Rhodes, Greece, September 3-7, **2006.**
91. G. Tsolou, **V.G. Mavrantzas**, "Atomistic molecular dynamics simulation of the temperature and pressure dependences of local and terminal relaxations in cis-1,4-polybutadiene", *4th International Workshop on Non-Equilibrium Thermodynamics and Complex Fluids (4th IWNET)*, Rhodes, Greece, September 3-7, **2006.**
92. V. Soni, J. Abildskov, G. Jonsson, R. Gani, N.Ch. Karayiannis, **V.G. Mavrantzas**, "Multiscale modeling property for design of polymer-based products", *AIChE Annual Meeting*, San Francisco, USA, Nov. 12 - 17, **2006.**
93. T. Ionescu, B.J. Edwards, D.J. Keffer, **V.G. Mavrantzas**, "Thermodynamics of non-isothermal polymer melts: Experiment, theory and simulation", *AIChE Annual Meeting*, San Francisco, USA, Nov. 12 - 17, **2006.**
94. R. Khare, O. Alexiadis, **V.G. Mavrantzas**, A. Baljon, "Monte Carlo simulations of the glass transition in polyethylene", *AIChE Annual Meeting*, San Francisco, USA, Nov. 12 - 17, **2006.**
95. O. Alexiadis, K.Ch. Daoulas, **V.G. Mavrantzas**, "An efficient Monte Carlo algorithm for the fast

equilibration and atomistic simulation of alkanethiol based self-assembled monolayers on a Au(111) substrate, *6th Hellenic Polymer Society Symposium (ELEP 2006)*, Patras, Greece, November 3-5, **2006**.

96. V. Dimitriadis, N.Ch. Karayiannis, **V.G. Mavrantzas**, E. Chiotellis, D. Mouratides, C.D. Kiparissides, "An advanced Monte Carlo algorithm for the fast thermal equilibration of polyethylene melts bearing short chain branches frequently spaced along their backbone (poster)", *6th Hellenic Polymer Society Symposium (ELEP 2006)*, Patras, Greece, November 3-5, **2006**.
97. R. Khare, O. Alexiadis, **V.G. Mavrantzas**, J. Beckers, A. Baljon, "Monte Carlo Simulation of the Glass Transition in Polyethylene", March 2007 Meeting of the Amer. Phys. Soc., Denver, Colorado, USA, March 5-9, **2007**.
98. C. Baig, **V.G. Mavrantzas**, "Thermodynamically guided atomistic simulation of polymer melts beyond equilibrium", *4th Annual European Rheology Conference (AERC-2007)*, Naples, Italy, April 12-14, **2007**.
99. O. Alexiadis, V.A. Harmandaris, **V.G. Mavrantzas**, L. Delle Site, "Atomistic simulation of alkanethiol self-assembled monolayers on different metal surfaces via a quantum, first-principles parameterization of the sulfur-metal interaction (poster)", *11th International Conference on Properties and Phase Equilibria (PPEPPD 2007)*, Hersonissos, Crete, Greece, May 20-25, **2007**.
100. G. Tsolou, **V.G. Mavrantzas**, "The temperature dependence of the Rouse mode relaxation spectrum and the zero shear rate viscosity of cis-1,4-polybutadiene: results from long atomistic molecular dynamics simulations down to the glass transition temperature (poster)", *11th International Conference on Properties and Phase Equilibria (PPEPPD 2007)*, Hersonissos, Crete, Greece, May 20-25, **2007.**
101. V. Soni, J. Abildskov, G. Jonsson, R. Gani, G. Tsolou, N.Ch. Karayiannis, **V.G. Mavrantzas**, "Integrating multilevel modelling aspects to predict gas permeability in polymers for the design of membranes (poster)", *11th International Conference on Properties and Phase Equilibria (PPEPPD 2007)*, Hersonissos, Crete, Greece, May 20-25, **2007.**
102. P.S. Stephanou, C. Baig, **V.G. Mavrantzas**, "Generalizing the Giesekus model so that it can account for chain finite-extensibility effects and analysis of its predictions for polymer melts in viscometric flows", *6thPanhellenic Chemical Engineers Conference*, Athens, Greece, May 31-June 2, **2007**.
103. G. Tsolou, **V.G. Mavrantzas**, "The temperature dependence of the Rouse mode relaxation spectrum and zero shear rate viscosity in cis-1,4-polybutadiene: Results from long atomistic molecular dynamics simulations down to the glass transition temperature, T_g (poster)", *XVth International Workshop on Numerical Methods for Non-Newtonian Flows (IWNMNNF 2007)*, Rhodes, Greece, June 6-10, **2007.**
104. P.S. Stephanou, C. Baig, **V.G. Mavrantzas**, "A generalized single-conformation tensor viscoelastic model based on principles of non-equilibrium thermodynamics (poster)", *XVth International Workshop on Numerical Methods for Non-Newtonian Flows (IWNMNNF 2007)*, Rhodes, Greece, June 6-10, **2007**.
105. C. Baig, **V.G. Mavrantzas**, "Atomistic Monte Carlo simulation of a polymer melt under a flow field by employing generalized ensembles", *XVth International Workshop on Numerical Methods for Non-Newtonian Flows (IWNMNNF 2007)*, Rhodes, Greece, June 6-10, **2007**.
106. G. Tsolou, **V.G. Mavrantzas**, "Atomistic molecular dynamics simulation of the static and dynamic properties of cis- and trans-1,4-polybutadiene systems over a wide range of temperature and pressure conditions", *2007 European Polymer Federation Congress (EPF 2007)*, Portorož-Portorose, Slovenia, July 2-6, **2007.**
107. G. Tsolou, **V.G. Mavrantzas**, "The effect of molecular architecture on the dynamic properties of polymers: atomistic MD simulations of cis- and trans-1,4-polybutadiene below and above the entanglement length", *2007 International Soft Matter Conference*, Aachen, Germany, October 1-4, **2007.**
108. G. Tsolou, **V.G. Mavrantzas**, "The temperature dependence of the Rouse relaxation spectrum and the zero shear rate viscosity of cis-1,4-polybutadiene: Results from long atomistic molecular dynamics simulations down to the glass transition temperature (poster)", *2007 International Soft Matter Conference*, Aachen, Germany, October 1-4, **2007.**
109. C. Baig, **V.G. Mavrantzas**, "Atomistic non-equilibrium molecular dynamics simulation of an H-

shaped polyethylene melt under shear", *The Society of Rheology 79th Annual Meeting (SOR 2007)*, Salt Lake City, Utah, USA, October 7-11, **2007**.

110. C. Baig, **V.G. Mavrantzas**, "Thermodynamically guided non-equilibrium Monte Carlo methodology for generating realistic shear flows of polymer melts", *The Society of Rheology 79th Annual Meeting (SOR 2007)*, Salt Lake City, Utah, USA, October 7-11, **2007**.
111. P.S. Stephanou, C. Baig, **V.G. Mavrantzas**, "A generalized, thermodynamically founded Giesekus model incorporating chain finite-extensibility and bounded free energy effects (poster)", *The Society of Rheology 79th Annual Meeting (SOR 2007)*, Salt Lake City, Utah, USA, October 7-11, **2007**.
112. O. Alexiadis, **V.G. Mavrantzas**, "Atomistic Monte Carlo simulation of alkanethiol self-assembled monolayers on different metal surfaces", *Condensed Matter Physics Conference of Balkan Countries,* Mugla University, Mugla, Turkey, May 26-28, **2008**.
113. C. Baig, **V.G. Mavrantzas**, "Thermodynamically guided nonequilibrium Monte Carlo method for generating realistic shear flows in polymeric materials", *The XVth International Congress on Rheology (ICR),* Monterey, California, USA, August 3-8, **2008**.
114. J.M. Kim, C. Baig, B.J. Edwards, D.J. Keffer, **V.G. Mavrantzas**, "Rheology of short-chain branched polyethylene melts under shear: Results from NEMD simulations and comparison with linear and H-shaped analogues", *The XVth International Congress on Rheology (ICR),* Monterey, California, USA, August 3-8, **2008**.
115. G. Tsolou, **V.G. Mavrantzas**, Z. Makrodimitri, I.G. Economou, "Atomistic simulation of the sorption of small gas molecules in polyisobutylene", *XXIV Panhellenic Conference on Solid State Physics and Materials Science*, Heraklion, Crete, September 24-27, **2008**.
116. P.S. Stephanou, C. Baig, G. Tsolou, **V.G. Mavrantzas**, M. Kröger, "Topological and Dynamical Mapping of atomistic simulation data onto the tube model for entangled polymer melts (poster)", *XXIV Panhellenic Conference on Solid State Physics and Materials Science*, Heraklion, Crete, September 24-27, **2008.**
117. G. Tsolou, **V.G. Mavrantzas**, A. Makrodimitri, I.G. Economou, "Atomistic simulation of the sorption of small gas molecules in polyisobutylene (poster)", *7th Panhellenic Conference on Polymers*, Ioannina, Greece, September 28-October 1, **2008**.
118. P.S. Stephanou, C. Baig, G. Tsolou, **V.G. Mavrantzas**, M. Kröger, "Topological and Dynamical Mapping of atomistic simulation data onto the tube model for entangled polymer melts", *7th Hellenic Polymer Society Symposium (ELEP 2008)*, Ioannina, Greece, September 28-October 1, **2008**.
119. P.S. Stephanou, C. Baig, G. Tsolou, **V.G. Mavrantzas**, M. Kröger, "Quantifying chain reptation in entangled polymers by mapping atomistic simulation results onto the tube model (poster)", *International Workshop on the Development and Analysis of Multiscale Methods,* Institute for Mathematics and its Applications (IMA), Minneapolis, Minnesota, USA*,* November 3-7, **2008**.
120. K.C. Satyanarayana, J. Abildskov, R. Gani, G. Tsolou, **V.G. Mavrantzas**, "Computer aided polymer design using multiscale modeling", *AIChE Annual Meeting*, Philadelphia, Nov. 16-21, **2008.**
121. K.C. Satyanarayana, J. Abildskov, R. Gani, G. Tsolou, **V.G. Mavrantzas**, "Atomistic Simulation of the Diffusion of Small Gas Molecules in polyisobutylene", *AIChE Annual Meeting*, Philadelphia, Nov. 16-21, **2008.**
122. C. Baig, **V.G. Mavrantzas**, "Multiscale simulation of polymer melt viscoelasticity guided from nonequilibrium statistical thermodynamics", *4th Annual European Rheology Conference (AERC-2009),* Edinburgh, U.K., April 14-17, **2009.**
123. C. Baig, P.S. Stephanou, **V.G. Mavrantzas**, "A generalized differential constitutive equation for polymer melts based on principles of nonequilibrium thermodynamics", *4th Annual European Rheology Conference (AERC-2009),* Edinburgh, U.K., April 14-17, **2009.**
124. G. Tsolou, P.S. Stephanou, C. Baig, **V.G. Mavrantzas**, M. Kröger, "Quantifying chain reptation in entangled polymer melts: Topological and dynamical mapping of atomistic simulation results onto the tube model", *4th Annual European Rheology Conference (AERC-2009),* Edinburgh, U.K., April 14-17, **2009.**
125. C. Baig, P.S. Stephanou, **V.G. Mavrantzas**, "Multiscale simulation of polymer melt viscoelasticity guided from nonequilibrium statistical thermodynamics: Atomistic nonequilibrium

thermodynamics coupled with Monte Carlo in an expanded statistical ensemble", *7th Panhellenic Chemical Engineers Conference*, Patras, Greece, June 3-5, **2009**.

126. P.S. Stephanou, C. Baig, G. Tsolou, **V.G. Mavrantzas**, M. Kröger, "Quantifying chain reptation in entangled polymer melts: Topological and dynamical mapping of atomistic simulation results onto the tube model", *7th Panhellenic Chemical Engineers Conference*, Patras, Greece, June 3-5, **2009**.
127. G. Tsolou, **V.G. Mavrantzas**, "Study of the unique dynamic, barrier and glass transition properties of polyisobutylene through detailed molecular dynamics simulations", *7th Panhellenic Chemical Engineers Conference*, Patras, Greece, June 3-5, **2009.**
128. C. Baig, O. Alexiadis, **V.G. Mavrantzas**, "Advanced Monte Carlo moves for the atomistic simulation of polymer melts with a variety of molecular architectures", *4th International Conference from Scientific Computing to Computational Engineering (4th IC-SCCE)*, Athens, Greece, July 7-10, **2010**.
129. P.S. Stephanou, C. Baig, G. Tsolou, **V.G. Mavrantzas**, "Mapping atomistic simulation results for the dynamics of entangled polymer melts onto the tube model of the reptation theory", *4th International Conference from Scientific Computing to Computational Engineering (4th IC-SCCE)*, Athens, Greece, July 7-10, **2010**.
130. C. Baig, P.S. Stephanou, G. Tsolou, **V.G. Mavrantzas**, "From atomistic trajectories to primitive paths to the reptation theory: Topological and dynamical mapping of molecular dynamics simulation data onto the tube model", *8th Hellenic Polymer Society Symposium (ELEP 2010)*, Hersonissos, Crete, October 24-29, **2010**.
131. G. Tsolou, N. Stratikis, C. Baig, P.S. Stephanou, **V.G. Mavrantzas**, "Melt Structure and Dynamics in melts of Unentangled Polyethylene Rings: Rouse Theory, Atomistic Molecular Dynamics Simulation, and Comparison with the Linear Analogues", *8th Hellenic Polymer Society Symposium (ELEP 2010)*, Hersonissos, Crete, October 24-29, **2010**.
132. C. Baig, P.S. Stephanou, G. Tsolou, **V.G. Mavrantzas**, "Quantitative analysis of segmental tube survival probabilities in entangled binary polymer mixtures from a direct mapping of atomistic MD simulation results onto the tube model", *AIChE Annual Meeting*, Salt Lake City, Utah, USA, Nov. 7-12, **2010.**
133. G. Tsolou, N. Stratikis, C. Baig, P.S. Stephanou, **V.G. Mavrantzas**, "Atomistic molecular-dynamics study of the structural and dynamical properties of unentangled polymer rings: Comprehensive analysis of the Rouse model and comparison with the simulation predictions", *AIChE Annual Meeting*, Salt Lake City, Utah, USA, Nov. 7-12, **2010.**
134. G.N. Nomikos, D.I. Kondarides, **V.G. Mavrantzas**, X.E. Verykios, "Photocatalytic reactor design for energy and environmental applications", *8th Panhellenic Chemical Engineers Conference*, Thessaloniki, Greece, May 26-28, **2011**.
135. G.N. Nomikos, D.I. Kondarides, **V.G. Mavrantzas**, X.E. Verykios, "Photocatalytic reactor design for energy and environmental applications", *2011 International Conference on H_2 production (ICH2P-2011)*, Thessaloniki, Greece, June 19-22, **2011**.
136. P.S. Stephanou, G. Tsolou, N. Stratikis, C. Baig, V.G. Mavrantzas, "Rouse theory for polymer rings and comparison with atomistic molecular-dynamics simulations", *6th International Meeting of the Hellenic Society of Rheology*, Athens, Greece, June 28-29, **2011.**
137. P.S. Stephanou, C. Baig, G. Tsolou, M. Kröger, V.G. Mavrantzas, "Quantifying chain reptation in entangled polymer melts: Topological and dynamical mapping of atomistic simulation results onto the tube model", *6th International Meeting of the Hellenic Society of Rheology (HSR 2011)*, Athens, Greece, June 28-29, **2011.**
138. A. Anastasiou, C. Baig, **V.G. Mavrantzas**, "Non-equilibrium Molecular Dynamics simulation of the stretching behavior of adhesive polymers", *6th International Meeting of the Hellenic Society of Rheology (HSR 2011)*, Athens, Greece, June 28-29, **2011.**
139. P.S. Stephanou, C. Baig, **V.G. Mavrantzas**, "Generalized viscoelastic model for polymer melts guided by principles of non-equilibrium thermodynamics: Single- and multi-mode formulations", *7th GRACM International Congress on Computational Mechanics (7th GRACM)*, Athens, Greece, June 30-July 2, **2011.**
140. A. Anastasiou, C. Baig, **V.G. Mavrantzas**, "Non-equilibrium molecular dynamics simulation of the stretching behavior of adhesive polymers", *7th GRACM International Congress on*

Computational Mechanics (7th GRACM), Athens, Greece, June 30-July 2, **2011.**

141. E. Karahaliou, O. Alexiadis, V.G. Mavrantzas, "Monte Carlo Simulation of Water Nanosorption in Carbon Nanotubes", *2011 International Conference on the Science and Application of Nanotubes (NT2011)*, Cambridge, UK, July 11-16, **2011**.
142. A. Anastassiou, C. Baig, **V.G. Mavrantzas**, "Non-equilibrium molecular dynamics simulation of the stretching behavior of adhesive polymers", *Thermodynamics 2011,* Athens, Greece, September 1-3, **2011.**
143. E. Karahaliou, O. Alexiadis, **V.G. Mavrantzas**, "Atomistic simulation of the nanosorption and nanofluidics of small molecules in carbon nanotubes", *Thermodynamics 2011,* Athens, Greece, September 1-3, **2011.**
144. P.S. Stephanou, C. Baig, **V.G. Mavrantzas**, "Quantifying chain reptation in entangled polymer melts: Topological and dynamical mapping of atomistic simulation results onto the tube model", *17th International Workshop on Numerical Methods for non-Newtonian flows (IWNMNNF 2012)",* Blois castle, France, March 25-28, **2012**.
145. P.S. Stephanou, C. Baig, **V.G. Mavrantzas**, "Quantifying chain reptation in entangled polymer melts: topological and dynamical mapping of atomistic simulation results onto the tube model", *The XVIth International Congress on Rheology (ICR 2012),* Lisbon, Portugal, August 5-10, **2012.**
146. **V.G. Mavrantzas**, P.S. Stephanou, N. Stratikis, T. Koukoulas, G. Tsolou, and C. Baig, "Rouse theory for polymer rings and comparison with atomistic molecular-dynamics simulations and experimental data", *The XVIth International Congress on Rheology (ICR 2012),* Lisbon, Portugal, August 5-10, **2012.**
147. C. Baig, P.S. Stephanou, **V.G. Mavrantzas**, "Quantifying chain reptation in entangled polymer melts: topological and dynamical mapping of atomistic simulation results onto the tube model", *The 23rd International Congress on Theoretical and Applied Mechanics (ICTAM 2012)*, Beijing, China, August 20-25, **2012**.
148. D. Tsalikis, C. Baig, **V.G. Mavrantzas**, L. Amanatidis, D. Mataras, "Hierarchical simulation of microcrystalline PECVD silicon film growth and structure", *13th International Conference on Plasma Surface Engineering (PSE 2012),* Garmisch-Partenkirchen, Germany, September 10 - 14, 2012.

149. D. Tsalikis, C. Baig, **V.G. Mavrantzas**, E. Amanatidis, D. Mataras, "Hierarchical simulation of microcrystalline silicon thin films growth and structure", Proceedings, *27th European Photovoltaic Solar Energy Conference and Exhibition (EU PSVEC 2012),* Messe Frankfurt, Germany, September 25-28, **2012**.

150. E. Karahaliou, A. Anastasiou, **V.G. Mavrantzas**, "Atomistic simulation of the nanosorption and nanofluidics of small molecules in carbon nanotubes", *GrapHEL Conference*, Mykonos, Greece, September 27-30, **2012**.
151. A. Anastasiou, M. Skountzos, S. Sabethai, **V.G. Mavrantzas**, "Molecular Dynamics simulation study of the structural and mechanical properties of graphene-based polymer nanocomposites", *GrapHEL Conference*, Mykonos, Greece, September 27-30, **2012**.
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, May 23-25, **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, May 23-25, **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, May 23-25, **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, May 25-27, **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, May 25-27, **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, May 25-27, **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, July 8-11, **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.S. 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, June 4-6, **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. 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 study and comparison with experimental data", *2nd Workshop of Graduates and Post-Doncs in Chemical Engineering Sciences,* Patras, Greece, September, **2016**.
205. 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**.

206. 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**.
207. 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**.
208. 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**.
209. 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**.
210. 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**.
211. 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**.
212. 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**.
213. V. Vasilev, E. Goudeli, E.N. Skountzos, **V.G. Mavrantzas**, S.E. Pratsinis, "Particle Collision Efficiency through Molecular Dynamics Simulations", *2016 MRS Fall Meeting & Exhibit*, Boston, USA, November 27 - December 2, **2016**.
214. 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**.
215. 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**.
216. A. Spyrogianni, K.S. Karadima, E. Goudeli, **V.G. Mavrantzas**, S.E. Pratsinis, "Brownian Dynamics simulation of the settling velocity of fractal nanoparticle agglomerates", *Swiss Association of Computational Chemistry (SACC) Meeting "Modeling and Simulation in Industrial Research" - Empa Akademie*, Dübendorf, Switzerland, February 09, **2017**.
217. 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**.
218. 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**.
219. 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**.
220. 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**.
221. 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**.
222. 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.**

223. A. Spyrogianni, K.S. 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.**
224. 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.**
225. 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.**
226. 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.**
227. 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.**
228. 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.**
229. 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.**
230. 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.**
231. 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.**
232. 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**.
233. 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**.
234. 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**.
235. 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.**
236. 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.**
237. 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.**
238. 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.**

239. 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**.
240. A. Spyrogianni, K.S. Karadima, E. Goudeli, **V.G. Mavrantzas**, S.E. Pratsinis, "Settling rate of nanosized fractal–like agglomerates by Brownian dynamics (BD) simulations", *European Aerosol Science Conference 2017 (EAC 2017)*, Zurich, Switzerland, August 27-September 01, **2017**.
241. E.N. Skountzos, **V.G. Mavrantzas**, S.E. Pratsinis, "Atomistic Monte Carlo simulation of the fractal dimensions of nanoparticle agglomerates", *European Aerosol Science Conference 2017 (EAC 2017)*, Zurich, Switzerland, August 27-September 01, **2017**.
242. 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**.
243. A. Spyrogianni, K.S. Karadima, E. Goudeli, **V.G. Mavrantzas**, S.E. Pratsinis, "Mobility and settling rate of fractal-like nanoaggregates: a Brownian Dynamics simulation study", *3rd Workshop of Graduates & Post-Docs in Chemical Engineering Sciences*, Patras, Greece, October 04, **2017**.
244. 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**.
245. 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**.
246. 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**.
247. **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**.
248. 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**.
249. 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**.
250. 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**.
251. 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**.
252. 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**.
253. T.S. Alexiou, D.G. Tsalikis, P.V. Alatas, **V.G. Mavrantzas**, "Atomistic simulation of DNA minicircles in aqueous solution", *4th Workshop of Graduates and Post-Docs in Chemical Engineering Sciences*, Patras, Greece, October 31, **2018**.
254. F.D. Tsourtou, K.S. Karadima, **V.G. Mavrantzas**, "Self-assembly in polypeptides with atomistic Monte Carlo", *4th Workshop of Graduates and Post-Docs in Chemical Engineering Sciences*,

Patras, Greece, October 31, **2018**.

255. D. Mintis, **V.G. Mavrantzas**, "Molecular dynamics simulation of the weak polyelectrolytes poly(ethylene-imine), poly(acrylic acid) and poly(N,N-dimethylaminoethyl methacrylate): Effect of salt, pH, temperature, branching and chain size", *4th Workshop of Graduates and Post-Docs in Chemical Engineering Sciences*, Patras, Greece, October 31, **2018**.
256. P. Mermigkis, E.N. Skountzos, **V.G. Mavrantzas**, "Conformational, dynamic, and permeability properties of atactic poly(methyl methacrylate) - carbon nanotube (PMMA-CNT) nanocomposites studied through molecular dynamics simulations", *4th Workshop of Graduates and Post-Docs in Chemical Engineering Sciences*, Patras, Greece, October 31, **2018**.
257. A.J. Tsamopoulos, D.G. Tsalikis, **V.G. Mavrantzas**, "Shear rheology of marginally entangled ring-linear poly(ethylene oxide) blends through nonequilibrium atomistic molecular dynamics simulations", *13th Annual European Rheology Conference (AERC-2019)*, Portorož, Slovenia, April 8-11, **2019**.
258. T. Alexiou, D.G. Tsalikis, P.V. Alatas, **V.G. Mavrantzas**, "Conformational and transport properties of DNA minicircles in dilute aqueous solutions: Detailed atomistic molecular dynamics simulation study", *12th Panhellenic Chemical Engineers Conference*, Athens, May 29-31, **2019**.
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**.
260. A.J. Tsamopoulos, A. Katsarou, D.G. Tsalikis, **V.G. Mavrantzas**, "Nonequilibrium molecular dynamics simulation of marginally entangled linear-ring polymer belnds", *12th Panhellenic Chemical Engineers Conference*, Athens, May 29-31, **2019**.
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 Conference*, Athens, May 29-31, **2019**.
263. A.F. Katsarou, A.J. Tsamopoulos, D.G. Tsalikis, **V.G. Mavrantzas**, "Dynamic heterogeneity ad topological intearctions in ring-linear polymer blends under flow (poster presentation)", *12th Panhellenic Chemical Engineers Conference*, Athens, May 29-31, **2019**.
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**.
265. T.S. Alexiou, E. Kriti, D. Loukas, **V.G. Mavrantzas**, "Atomistic molecular dynamics simulation of the diffusion dynamics of short linear DNA molecules: comparison with experimental data and theoretical models (poster presentation)", *Frontiers in Polymer Science 2019*, Budapest, Hungary, June 05-08, **2019**.
266. T.S. Alexiou, D.G. Tsalikis, P.V. Alatas, **V.G. Mavrantzas**, "Conformational and transport properties of small circular and linear DNA molecules in dilute solution: A detailed molecular dynamics simulations study", *European Polymer Congress* (*EPF 2019)*, Hersonissos Heraklion Crete, Greece, June 9-14, **2019**.
267. D.G. Tsalikis, P.V. Alatas, T.S. Alexiou, **V.G. Mavrantzas**, "Shear rheology of marginally entangled ring polymer melts through non-equilibrium atomistic molecular dynamics simulations", *European Polymer Congress* (*EPF 2019)*, Hersonissos Heraklion Crete, Greece, June 9-14, **2019**.
268. D.G. Tsalikis, E.N. Skountzos, P.S. Stephanou, **V.G. Mavrantzas**, "On the role of chain end-functional groups on microscopic structure and dynamics of polymer nanocomposites (poster presentation)", *European Polymer Congress* (*EPF 2019)*, Hersonissos Heraklion Crete, Greece, June 9-14, **2019**.
269. D.G. Tsalikis, A.J. Tsamopoulos, A. Katsarou, **V.G. Mavrantzas**, "Steady shear flow of marginally entangled ring polymer melts through nonequilibrium molecular dynamics simulations", *9th International Meeting of the Hellenic Society of Rheology (HSR 2019)*, Pythagorion, Samos, Greece, June 23-27, **2019**.

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**.
271. D.G. Mintis, **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)", *International Conference on Adhesion in Aqueous Media: From Biology to Synthetic Materials (AAM2019)*, Dresden, Germany, September 9-12, **2019**.
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**.
291. 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**.
292. E.N. Skountzos, D.G. Tsalikis, P.S. Stephanou, **V.G. Mavrantzas**, "Individual contributions of adsorbed and free chains to microscopic dynamics of unentangled poly(ethylene glycol) - silica nanocomposite melts and the important role of end groups: Theory and Simulation", *13th Hellenic Polymer Siociety Conference (ELEP 2021, virtual event),* Athens, Greece, December 12-16*,* **2021**.
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**.
316. E.N. Skountzos, D.G. Tsalikis, P.S. Stephanou, **V.G. Mavrantzas**, "A combined theoretical-simulation approach to microstructure and dynamics of unentangled poly(ethylene glycol) - silica nanocomposite melts", *XIXth International Congress on Rheology (ICR2023)*, Athens, Greece, July 29 – August 4, **2023**.
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**.

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).
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).
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).

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**.
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: 55%, 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 (2024 – to date)
46. Efi Lepenioti (2024 – to date)
47. Aristeidis Koukoutsis (2025 – to date)
48. Athina Spyropoulou (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 (2023 – to date)

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 (2020 – to date) (jointly with Prof. S.N. Pandis)
12. Panagiotis Panagopoulos Papageorgiou (2023 – to date)
13. 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 – todate)
10. Katerina Karadima (2013 – todate)
11. Pavlos Stephanou (2017 – 2019)
12. Stavros Peroukidis (2017 – 2020)
13. Terpsichori Alexiou (2017 – 2021)

14. Emmanouil Symianakis (2018 – 2020)
15. George Leonis (2023 – to date)
16. Georgios Vogiatzis (2025 – to date)

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)

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 - to date)
3. Dr. Dimitrios Tsalikis (co-advised with Prof. S.E. Pratsinis, 2023 - to date)

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

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