VLASIS G. MAVRANTZAS

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71. F.D. Tsourtou, **V.G. Mavrantzas**, "Atomistic Monte Carlo and Molecular Dynamics simulation of

nanostructured semiconducting polymers and polypeptides", *11th Panhellenic Chemical Engineers Conference*, Salonica, Greece, May 25-27, **2017.**

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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)

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rheology of polymer solutions", *March Meeting of the American Physical Society*, Cincinnati, March 18-22, **1991**.

2. **V.G. Mavrantzas**, A.N. Beris, "Theoretical study of the effects of solid/fluid interface on the rheology of polymer solutions", *"Symposium on Interfacial Phenomena in Viscoelastic Flows*" organized by the Fluid Mechanics Committee of the Applied Mechanics Division of ASME, Columbus, June 16-19, **1991**.
3. **V.G. Mavrantzas**, A.N. Beris, "Theoretical Study of wall effects on the rheology of dilute polymer solutions", *Society of Rheology Meeting*, Rochester, October 20-24, **1991**.
4. **V.G. Mavrantzas**, A.N. Beris, "Modeling and simulation of the dilute polymer solution flow behavior next to solid surfaces and interfaces", *National Meeting of the American Chemical Society*, San Francisco, April 5-10, **1992**.
5. **V.G. Mavrantzas**, A.N. Beris, "Interfacial phenomena in the rheology of dilute polymer solutions", *AIChE Annual Meeting*, Miami Beach, November 1-6, **1992**.
6. A.N. Beris, **V.G. Mavrantzas**, "Non-local effects in polymer rheology: Polymer-surface interactions", *Society of Rheology Meeting*, Boston, October 17-21, **1993**.
7. **V.G. Mavrantzas**, A.N. Beris, "Stress-induced polymer migration phenomena in simple viscometric flows", *Society of Rheology Meeting*, Boston, October 17-21, **1993**.
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10. **V.G. Mavrantzas**, D.N. Theodorou, "From chain chemical structure to polymer melt elasticity: The implementation of new Monte Carlo techniques'', *EPF Annual Meeting*, Aghia Pelaghia, Crete, Greece, October 7-11, **1996**.
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12. V.A. Harmandaris, **V.G. Mavrantzas**, D.N. Theodorou, "From chemical structure to polymer processing: Atomistic simulation of the viscoelasticity of linear polyethylene melts", *4th Hellenic Polymer Society Symposium (ELEP 1997)*, Patras, Greece, November 20-22, **1997**.
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14. E. Zervopoulou, **V.G. Mavrantzas**, D.N. Theodorou, "Atomistic simulation of the solubility of small alkanes in long polyethylene melts", *2nd Panhellenic Chemical Engineers' Conference*, Salonica, Greece, May 27-29, **1999**.
15. V.A. Harmandaris, **V.G. Mavrantzas**, D.N. Theodorou, "Atomistic simulation of the stress relaxation experiment after cessation of steady-state uniaxial elongation", *2nd Panhellenic Chemical Engineers' Conference*, Salonica, Greece, May 27-29, **1999**.
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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.**
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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**.
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38. K.Ch. Daoulas, **V.G. Mavrantzas**, V.A. Harmandaris, K. Foteinopoulou, D.N. Theodorou, "Atomistic Monte Carlo simulations and SCF Calculations of polymers at interfaces"*, 4th GRACM Congress on Computational Mechanics*, Patras, Greece, June 27-29, **2002**.
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*

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48. **V.G. Mavrantzas**, "Thermodynamically founded hierarchical methodologies for the simulation of polymer melts beyond equilibrium: Detailed atomistic simulation of polymer melt viscoelasticity", *3rd International Workshop on Non-Equilibrium Thermodynamics and Complex Fluids (3rd IWNET)*, Princeton, USA, August 14-17, **2003**.
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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**.
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261. D.G. Mintis, D. Rigou, **V.G. Mavrantzas**, "Detailed molecular dynamics simulation study of the phase boundary for complex coacervation between poly(acrylic acid) and poly(N,N-dimethyl amino ethyl methacrylate) (poster presentation)", *12th Panhellenic Chemical Engineers Conference*, Athens, May 29-31, **2019**.
262. T. Alexiou, E. Kriti, D. Loukas, **V.G. Mavrantzas**, "Atomistic molecular dynamics simulation of the diffusive behavior of short linear DNA molecules in dilute aqueous solutions: Comparison with experiments and theoretical models (poster presentation)", *12th Panhellenic Chemical Engineers Conference*, Athens, May 29-31, **2019**.
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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**.
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270. P.S. Stephanou, I.Ch. Tsimouri, G.C. Georgiou, **V.G. Mavrantzas**, "Understanding the rheological behaviour of blood from a non-equilibrium thermodynamics perspective", *9th International Meeting of the Hellenic Society of Rheology (HSR 2019)*, Pythagorion, Samos, Greece, June 23-27, **2019**.
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**.
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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**.
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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**.