VLASIS G. MAVRANTZAS

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BOOKS Edited

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   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: Field theoretic approaches to polymer and copolymer systems
Chapter 10: Dissipative Particle Dynamics
Chapter 11: Introduction to Beyond-Equilibrium Thermodynamics

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PRESENTATIONS (speaker underlined)

1. **V.G. Mavrantzas**, A.N. Beris, "Theoretical study of the effects of solid/fluid interface on the rheology of polymer solutions", *March Meeting of the American Physical Society*, Cincinnati, March 18-22, **1991**.
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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**.
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208. D.G. Tsalikis, **V.G. Mavrantzas**, D. Vlassopoulos, "Geometric analysis of threading events in melts of ring polymers and their connection with the slow relaxation modes", *11th Hellenic Polymer Society Conference (ELEP 2016)*, Heraklion, Crete, Greece, November 3-5, **2016**.
209. I.Ch. Tsimouri, Ch.K. Georgantopoulos, P.S. Stephanou, **V.G. Mavrantzas**, "Derivation of a recently proposed CCR model through the use of non-equilibrium thermodynamics", *11th Hellenic Polymer Society Conference (ELEP 2016)*, Heraklion, Crete, Greece, November 3-5, **2016**.
210. F.D. Tsourtou, **V.G. Mavrantzas**, "Atomistic Monte Carlo and Molecular Dynamics Algorithms for the simulation of self-assembly in soft matter", *11th Hellenic Polymer Society Conference (ELEP 2016)*, Heraklion, Crete, Greece, November 3-5, **2016**.
211. E.N. Skountzos, **V.G. Mavrantzas**, S.E. Pratsinis, "From atoms to primary particles to agglomerates: Hierarchical modeling of the fractal dimensions of nanoparticles", *2016 MRS Fall Meeting & Exhibit*, Boston, USA, November 27 - December 2, **2016**.
212. E.N. Skountzos, **V.G. Mavrantzas**, C. Tsitsilianis, "Atomistic simulation of pyrene functionalized α,ω-PMMA as dispersing agent of graphene for the fabrication of polymer nanocomposites", *2016 MRS Fall Meeting & Exhibit*, Boston, USA, November 27 - December 2, **2016**.
213. D.G. Tsalikis, E.N. Skountzos, **V.G. Mavrantzas**, "Computational study of microscopic dynamics in Polyethylene Glycol melts filled with Silica Nanoparticles and comparison with experimental data", *2016 MRS Fall Meeting & Exhibit*, Boston, USA, November 27 - December 2, **2016**.
214. P.S. Stephanou, D.G. Tsalikis, P.V. Alatas, **V.G. Mavrantzas**, "Multiscale modelling approach to the rheological behaviour of polymer nanocomposites: Nonequilibrium thermodynamics modelling coupled with NEMD simulations", *11th Annual European Rheology Conference (AERC-2017)*, Copenhagen, Denmark, April 3-6, **2017**.
215. I.Ch. Tsimouri, C.K. Georgantopoulos, P.S. Stephanou, **V.G. Mavrantzas**, "Derivation of a recently proposed CCR model through the use of non-equilibrium thermodynamics", *11th Annual European Rheology Conference (AERC-2017)*, Copenhagen, Denmark, April 3-6, **2017**.
216. D.G. Tsalikis, G.D. Papadopoulos, **V.G. Mavrantzas**, "Microscopic dynamics and topology of polymer rings immersed in a host matrix of longer linear polymers: Results from a detailed molecular dynamics simulation study and comparison with experimental data", *PRACE Scientific and Industrial Conference (PRACEdays17)*, Barcelona, Spain, May 16-18, **2017**.
217. F. Tsourtou, **V.G. Mavrantzas**, "Optimized Monte Carlo and Molecular Dynamics algorithms for modelling the self-organization of two classes of materials: semifluorinated alkanes and

semiconducting polymers based on thiophenes", *PRACE Scientific and Industrial Conference (PRACEdays17)*, Barcelona, Spain, May 16-18, **2017**.

218. E.N. Skountzos, **V.G. Mavrantzas**, "Atomistic simulation of pyrene functionalized α,ω-PMMA as dispersing agent of graphene for the fabrication of polymer nanocomposites", *PRACE Scientific and Industrial Conference (PRACEdays17)*, Barcelona, Spain, May 16-18, **2017**.
219. P.V. Alatas, D.G. Tsalikis, **V.G. Mavrantzas**, "Molecular dynamics simulation of the differences in the conformational and dynamic properties between and linear polyethylene oxide melts in the crossover region from unentangled to entangled", *11th Panhellenic Chemical Engineers Conference*, Salonica, Greece, May 25-27, **2017.**
220. A. Spyrogianni, K.K. Karadima, E. Goudeli, **V.G. Mavrantzas**, S.E. Pratsinis, "Brownian dynamic simulation of the settling rate of fractal-like nanoparticle agglomerates", *11th Panhellenic Chemical Engineers Conference*, Salonica, Greece, May 25-27, **2017.**
221. D. Mallios, D.G. Tsalikis, **V.G. Mavrantzas**, "Self-assembly of amphiphile peptides into nanostructures through detailed molecular dynamics simulations", *11th Panhellenic Chemical Engineers Conference*, Salonica, Greece, May 25-27, **2017.**
222. P. Mermigkis, E.N. Skountzos, **V.G. Mavrantzas**, "Study of water molecule mobility in carbon nanotubes embedded in a PMMA matrix", *11th Panhellenic Chemical Engineers Conference*, Salonica, Greece, May 25-27, **2017.**
223. D. Mintis, P.V. Alatas, D.G. Tsalikis, **V.G. Mavrantzas**, "Conformational transition of poly(ethylene-imine) in aqueous solution at different protonation states and its role in the formation of complex coacervate elucidated from Atomistic Molecular Dynamics Simulations", *11th Panhellenic Chemical Engineers Conference*, Salonica, Greece, May 25-27, **2017.**
224. C.K. Georgantopoulos, I.Ch. Tsimouri, P.S. Stephanou, **V.G. Mavrantzas**, "Development of state-of-the-art constitutive rheological models for entangled polymeric fluids using principles of nonequilibrium thermodynamics",*11th Panhellenic Chemical Engineers Conference*, Salonica, Greece, May 25-27, **2017.**
225. E.N. Skountzos, D.G. Tsalikis, **V.G. Mavrantzas**, "On the effect of end-functionalized groups on the dynamics of polymer melt nanocomposites through molecular dynamics simulations", *11th Panhellenic Chemical Engineers Conference*, Salonica, Greece, May 25-27, **2017.**
226. P.S. Stephanou, D.G. Tsalikis, E.N. Skountzos, **V.G. Mavrantzas**, "Modelling of polymer nanocomposite melts based on principles of nonequilibrium thermodynamics and on the findings of detailed nonequilibrium molecular dynamics simulations", *11th Panhellenic Chemical Engineers Conference*, Salonica, Greece, May 25-27, **2017.**
227. I.Ch. Tsimouri, P.S. Stephanou, **V.G. Mavrantzas**, "A constitutive rheological model for the blodod from nonequilibrium thermodynamics", *11th Panhellenic Chemical Engineers Conference*, Salonica, Greece, May 25-27, **2017.**
228. F.D. Tsourtou, **V.G. Mavrantzas**, "Atomistic Monte Carlo and Molecular Dynamics simulation of nanostructured semiconducting polymers and polypeptides", *11th Panhellenic Chemical Engineers Conference*, Salonica, Greece, May 25-27, **2017.**
229. E.N. Skountzos, D.G. Tsalikis, **V.G. Mavrantzas**, "Molecular simulation of PMMA-graphene and PEO-silica polymer nanocomposites in full atomistic detail", *SCIMEETING Europe, Materials Modellig and Simulations Conference*, Athens, Greece, June 21-23, **2017**.
230. F. Tsourtou, S. Peroukidis, and **G. Mavrantzas**, "Monte Carlo and Molecular Dynamics simulation of liquid-crystalline phases of oligothiophenes using a united-atom model", *14th European Conference on Liquid Crystals (ECLC 2017)*, Moscow, Russia, June 24-30, **2017**.
231. K.S. Karadima, **V.G. Mavrantzas**, S.N. Pandis, "The effect of organics and humidity on the structure of atmospheric nanoparticles: A molecular dynamics simulation study", *20th International Conference on Nucleation and Atmospheric Aerosols (ICNAA 2017)*, Helsinki, Norway, June 25-39, **2017**.
232. P.S. Stephanou, D.G. Tsalikis, E.N. Skountzos, **V.G. Mavrantzas**, "Multiscale modelling approach to the rheological behaviour of polymer nanocomposites: Nonequilibrium thermodynamics modelling coupled with NEMD simulations", *8th International Meeting of the Hellenic Society of Rheology (HSR 2017)*, Limassol, Cyprus, July 12-14, **2017.**
233. D.G. Tsalikis, P.V. Alatas, **V.G. Mavrantzas**, "Ring polymers: scaling laws and topological interactions based on detailed molecular dynamics simulations", *8th International Meeting of the*

Hellenic Society of Rheology (HSR 2017), Limassol, Cyprus, July 12-14, **2017.**

234. P.S. Stephanou, **V.G. Mavrantzas**, "Multi-scale modelling of high-MW polymer melt viscoelasticity starting from the atomistic level", *8th International Meeting of the Hellenic Society of Rheology (HSR 2017)*, Limassol, Cyprus, July 12-14, **2017.**
235. I.Ch. Tsimouri, C.K. Georgantopoulos, P.S. Stephanou, **V.G. Mavrantzas**, "Derivation of a recently proposed CCR model through the use of non-equilibrium thermodynamics", *8th International Meeting of the Hellenic Society of Rheology (HSR 2017)*, Limassol, Cyprus, July 12-14, **2017.**
236. K.S. Karadima, **V.G. Mavrantzas**, S.N. Pandis, "Molecular dynamics simulation of atmospheric nanoparticles: local structure and morphology", *European Aerosol Conference (EAC 2017)*, Zurich, Switzerland, August 27-September 01, **2017**.
237. D.G. Tsalikis, **V.G. Mavrantzas**, "Microscopic dynamics and topology of polymer rings immersed in a host matrix of longer linear polymers: Results from a detailed molecular dynamics simulation study and comparison with experimental data", *Ring Polymers: Focused Workshop*, Heraklion, Crete, September 25-27, **2017**.
238. A. Spyrogianni, K.S. Karadima, E. Goudeli, **V.G. Mavrantzas**, S.E. Pratsinis, "Mobility and Sedimentation of Agglomerates with Polydisperse Primary Particles", *2017 Conference of the Americal Association for Aerosol Research (2017 AAAR)*, Raleigh, North Carolina, October 16-20, **2017**.
239. A. Spyrogianni, K.S. Karadima, E. Goudeli, **V.G. Mavrantzas**, S.E. Pratsinis, "Sedimentation of Agglomerates Consisting of Polydisperse Nanoparticles", *AIChE Annual Meeting*, Minneapolis, USA, October 29 - November 03, **2017**.
240. A. Spyrogianni, K.S. Karadima, E. Goudeli, **V.G. Mavrantzas**, S.E. Pratsinis, "Settling rate of agglomerates consisting of polydisperse primary particles by Brownian Dynamics", *AIChE Annual Meeting*, Minneapolis, USA, October 29 - November 03, **2017**.
241. D.G. Tsalikis, **V.G. Mavrantzas**, "Melt rheology of ring poly(ethylene oxide) melts and comparison with experimental data", *12th Annual European Rheology Conference (AERC-2018)*, Sorrento, Italy, April 17-20, **2018**.
242. **V.G. Mavrantzas**, P.V. Alatas, H.C. Öttinger, "Third-order perturbation expansion of the two-point correlation function of the dissipative quantum φ^4 theory", *8th International Workshop on Non-equilibrium Thermodynamics and Complex Fluids (IWNET 2018)*, Sint-Michielsgestel, The Netherlands, July 1-6, **2018**.
243. D. Mintis, **V.G. Mavrantzas**, "Atomistic molecular dynamics simulation of weak polyelectrolytes in water", *12th International Symposium on Polyelectrolytes (ISP2018)*, Wageningen, The Netherlands, August 26-31, **2018**.
244. F.D. Tsourtou, K. Kardima, **V.G. Mavrantzas**, "Atomistic Monte Carlo: A powerful technique for simulating self-assembly in polypeptides", *BioExcel 2nd SIG Meeting: "Advanced Simulations for Biomolecular Research" @ ECCB 2018*, Athens, Greece, September 8, **2018**.
245. T.S. Alexiou, D.G. Tsalikis, P.V. Alatas, **V.G. Mavrantzas**, "Conformational and dynamic properties of DNA minicircles in aqueous solution from atomistic molecular dynamics simulations", *12th Hellenic Polymer Society International Conferemce (ELEP 2018)*, Ioannina, Greece, September 30-October 3, **2018**.
246. P.G. Mermigkis, E.N. Skountzos, **V.G. Mavrantzas**, "Conformational, dynamic, and permeability properties of atactic poly(methyl methacrylate) - carbon nanotube (PMMA-CNT) nanocomposites from molecular simulations", *12th Hellenic Polymer Society International Conferemce (ELEP 2018)*, Ioannina, Greece, September 30-October 3, **2018**.
247. D.G. Tsalikis, **V.G. Mavrantzas**, "Conformation and dynamics of ring polymers in dilute solutions of linear matrices: Results from a systematic molecular dynamics simulation study and comparison with experimental data", *12th Hellenic Polymer Society International Conferemce (ELEP 2018)*, Ioannina, Greece, September 30-October 3, **2018**.

INVITED LECTURES

1. "*Atomistic simulation of the viscoelasticity of unentangled polymer melts*", Institute for Polymers, Department of Materials, ETH, Zürich, Switzerland, February **2000**.
2. "*Modeling the rheology of polymer melts through multiscale modeling*", Dow Chemicals, Midland,

December **2000**.

3. "*Hierarchical modeling of the rheology of polymer melts*", CECAM-SIMU Workshop, Multiscale Modeling of Materials, Heraklion, Crete, July **2001**.
4. *"Atomistic simulation of polymer melts off equilibrium using principles of irreversible thermodynamics"*, CPERI-CERTH, Salonica, October **2001**.
5. *"Molecular simulations of polymers with emphasis on their viscoelasticity*", 5th Panhellenic Conference on Polymers, Heraklion, Crete, December 15-17, **2001**.
6. *"A hierarchical model for the rheology of polymers in confined geometries",* Institute for Polymers, Department of Materials, ETH, Zürich, Switzerland, February **2002**.
7. "*Polymer melts grafted on a solid substrate or graphite: Detailed atomistic simulation of their interfacial properties and ^{2}H-NMR spectrum*", XVIII Panhellenic Conference on Solid State Physics-Materials Science, Heraklion, Crete, September 15-18, **2002**.
8. "*Atomistic simulations of polymers at multiple time and length scales*", Max-Planck Institute for Polymer Research (MPI-P), Mainz, Germany, March **2003**.
9. "*Hierarchical modelling of polymers with a non-linear molecular architecture: Calculation of branch point friction and chain reptation time of an H-shaped polyethylene melt from detailed atomistic simulations*", 1st Mainz Materials Simulation Days (MMSD 2005), Max-Planck Institute for Polymer Research (MPI-P), Mainz, Germany, June 8-10, **2005**.
10. "*Hierarchical modelling of polymers with a non-linear molecular architecture: Calculation of branch point friction and chain reptation time of an H-shaped polyethylene melt from detailed atomistic simulations*", Japan Society of Technology (JST) Symposium: "Towards Multi-scale Modeling in Soft Matter", Tokyo, Japan, June 21-22, **2005**.
11. *Multi-scale modelling of polymers with a non-linear molecular architecture*", Keynote lecture, International Workshop on Mesoscale and Multiscale Description of Complex Fluids, Prato, Italy, July 5-8, **2006**.
12. "*Simulation of polymers with a non-linear molecular architecture*", ΕΚΕΤΑ-ΙΤΧΗΔ, February 3, **2006**.
13. "*Multi-scale modeling of polymers with a non-linear molecular architecture*", Keynote lecture, International Workshop on Mesoscale and Multiscale Description of Complex Fluids, Prato, Italy, July 5-8, **2006**.
14. *"Thermodynamically guided atomistic Monte Carlo simulation of polymer melts beyond equilibrium",* International Workshop on Multi-scale Modeling and Simulation of Complex Fluids, Maryland, USA, April 13-19, **2007.**
15. *"Polymer melt viscoelasticity: What can we learn from molecular simulations",* Department of Materials Science, University of Crete, Heraklion, Crete, May 25, **2007**.
16. *"Polymer melt viscoelasticity: What can we learn from molecular simulations",* Department of Applied Physics, University of Eindhoven, Eindhoven, The Netherlands, October 1, **2007**.
17. *"Hierarchical Modeling of Polymers: From the atomistic to the meso- to the macro-scale",*ENPC, Paris, November 26, **2007**.
18. *"Modeling in nanomaterials: The Monte Carlo Method",* International school on Nanostructure materials and membranes modeling and simulation, FORTH-ICE/HT, Patras, June 18-27, **2008**.
19. *"Atomistic Monte Carlo methodology for generating realistic flows of polymers guided by principles of non-equilibrium thermodynamics",* Polymer Physics Gordon Conference, Salve Regina University, Rhode Island, USA, June 29 - July 4, **2008.**
20. *"Hierarchical modeling of polymers at equilibrium and beyond-equilibrium conditions with emphasis on their mechanics and viscoelasticity",* DSM-Sabic R&D, The Netherlands, September 26, **2008**.
21. "*Hierarchical modeling of polymers at equilibrium and beyond equilibrium conditions with emphasis on viscoelasticity*", International seminar on Multi-scale modeling and simulation, Trondheim, Norway, October 13-14, **2008**.
22. "*Multiscale simulation of polymer melt viscoelasticity guided from non-equilibrium statistical thermodynamics: Atomistic Non-Equilibrium Molecular Dynamics coupled with Monte Carlo in an expanded statistical ensemble*", 6th International Discussion Meeting on Relaxations in Complex Systems, Rome, Italy, August 30 - September 5, **2009**.
23. "*Quantifying chain reptation in entangled polymer melts: Topological and dynamical mapping of*

atomistic simulation results onto the tube model", Theory and Computer Simulation of Polymers", Moscow, Russia, May 31 - June 6, **2010**.

24. *"Modeling polymer melt viscoelasticity: Quantifying chain reptation in entangled polymer melts through a novel topological and dynamical mapping of atomistic simulation results onto the tube model*", International Workshop on Novel Simulation methods in Soft matter Systems (NSASM-2010)", Dresden, Germany, September 20-24, **2010**.
25. *"Atomic and electronic structure of polymer organic semiconductors: What we can learn from computer simulations at different scales*", 9th Hellenic Polymer Society Symposium (ELEP 2012), Thessaloniki, Greece, November 29-December 01, **2012**.
26. *"Interfacing molecular simulations with theories of polymer dynamics: the case of entangled polymer melts and polymer rings",* Department of Materials Science, University of Crete, Heraklion, Crete, March 01, **2013**.
27. *"Topological interactions in ring poly(ethylene oxide) melts and their correlation with conformational and rheological properties: A computer simulation study",* Ring Polymers: Advances and Applications, Heraklion, Crete, July 12-15, **2015**.
28. *Simulation of polymer melts beyond equilibrium using a non-dynamic method (GENERIC Monte Carlo) in an expanded ensemble*, Technical University of Eindhoven, Department of Mechanical Engineering, April 19, **2016.**
29. *Using nonequilibrium thermodynamics to extend atomistic Monte Carlo simulations of polymers beyond equilibrium*, Multiscale Simulation Methods for Soft Matter Systems, Darmstadt, Germany, October 4-6, **2016**.
30. *Atomistic Monte Carlo simulation of self-assembly in soft matter systems*, SCIMEETING Europe, Materials Modellig and Simulations Conference, Athens, Greece, June 21-23, **2017**.
31. *Fundamentals of Molecular Simulations*, Advances in the Mechanics and Chemistry of Adshesion: Training School in the course of the European Marie-Curie Training Project BioSmartTrainee, Paris, France, September 13-15, **2017**.
32. *Microscopic dynamics and threadings in ring polymers: A detailed computer simulation study*, Ring Polymers: Focused Workshop, Heraklion, Crete, September 25-27, **2017**.
33. *Molecular modelling of materials: making a difference in industry*, Plastics Update, 2nd edition, Fribourg, Switzerland, November 9, **2017**.
34. *Topological constraimts in ring polymers*, 12th Hellenic Polymer Society Symposium (ELEP 2018), Ioannina, Greece, September 30 – October 03, **2018**.