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PRESENTATIONS (speaker underlined)

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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.C. 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**.

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, April 19, **2016.**
29. *Using nonequilibrium thermodynamics to extend atomistic Monte Carlo simulations of polymers beyond equilibrium,* Darmstadt University, October 4-6, **2016**.