

DIMITRIOS G. TSALIKIS

Birth date: 19 August 1980
Married, 2 children

Current position: Post-doctoral research Fellow, Department of Chemical Engineering, University of Patras

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Military service: Fulfilled (8/2009 - 4/2010)

Research experience

- 2011- Post-doctoral research fellow, Department of Chemical Engineering, University of Patras
- 11-12/2008: Visiting student, CINECA Supercomputing Centre, Bologna, Italy, (HPC Europa2 mobility program)
- 1-2/2008: Visiting student, Barcelona Supercomputing Centre, Barcelona, Spain, (HPC Europa++ mobility program)
- 1-2/2007: Visiting student, CINECA Supercomputing Centre, Bologna, Italy, (HPC Europa mobility program)
- 2005-2009: PhD dissertation «Computational study of structural relaxation and plastic deformation of glassy polymers», School of Chemical Engineering National Technical University of Athens (NTUA)

Education

- Diploma in Chemical Engineering, University of Patras, 2004 (GPA: 6.98/10.00)
- Ph.D., School of Chemical Engineering, NTUA, 2009, PhD thesis title: « Computational study of structural relaxation and plastic deformation of glassy polymers », under the supervision of Prof. Doros N. Theodorou

Teaching activities

- 2005-2009: Teaching Assistant, Laboratory of Physical Chemistry, NTUA
- 2014-15 & 2016-17: Instructor, course: *Rheology of Polymers*, Interdisciplinary Graduate Program of Studies, “Polymer Science and Technology”, University of Patras

Student co-supervision (with italics the ongoing student supervisions)

- In collaboration with Prof. Doros Theodorou, School of Chemical Engineering, NTUA: Nikolaos Lempesis (diploma thesis)
- In collaboration with Prof. Vlasios Mavrantzas, Department of Chemical Engineering, University of Patras:
 - Diploma thesis: Andreas Doukas, Eirini Goudeli, Ioanna Mavrikou, Aggeliki Chatzintouna, Apostolos Ziovas, Nikoletta Alexaki, Artemis Charalampidou, Dimitris Mallios, *Eleni Chousa*, *Konstantinos Papadopoulos*, *Georgios Zygouris*, *Alexandros Tsamopoulos*
 - Master thesis: Panagiotis Memrigkis, Georgios Papadopoulos, *Dimitris Mallios*
 - PhD student: *Panagiotis Alatas*
- In collaboration with Prof. Vlasios Mavrantzas and Prof. Sotiris Pratsinis, Department of Mechanical and Process Engineering, ETH Zurich: Saskia Kohler (bachelor’s thesis)

Professional activities

- Reviewer for *Soft Matter* (Royal Society of Chemistry) and *Plasma Process and Polymers* (Wiley)

- American Chemical Society, regular fellow
- PRACE Expert

Awards, Honors, Fellowships

- *Best Poster Award*, 11th Hellenic Polymer Society International Conference POLYCONF11, Heraklion, Greece (2016)
- *Best Poster Award*, 2nd Workshop of Graduates and Post-Docs in Chemical Engineering Sciences (CES-WGP2), FORTH-ICE/HT, Patras, Greece (2016)
- *PRACE DECI-12 Award*: Allocation of 1.500.000 CPU hours by PRACE (2014)
- *LinkSCEEM fellowship*: Fellowship to attend Second LinkSCEEM General User Meeting organized by The Cyprus Institute in Nicosia, Cyprus (2012)
- *PRACE DECI-9 Award*: Allocation of 7.200.000 CPU hours by PRACE (2012)
- *HPC Europa 2*: Financial support for research visit in Barcelona Supercomputing Centre Barcelona, Spain (2009)
- *HPC Europa++*: Financial support for research visit in CINECA Supercomputing Centre Bologna, Italy (2008)
- *Marie Curie Action* to attend "School on Understanding Molecular Simulations", University of Amsterdam, The Netherlands (2008)
- *HPC Europa*: Financial support for research visit in CINECA Supercomputing Center Bologna, Italy (2007).

Computer skills

- Administration: Cluster Rocks 6.6
- Programming: FORTRAN, MPI
- Modelling software: GROMACS, LAMMPS, NAMD, Scienomics MAPS, Wolfram Mathematica

Participation in the following Research Projects:

MMM@HPC

- EC (FP7-INFRA-2010-1.2.2) project titled: *Multiscale materials modeling on high performance computing (MMM@HPC)*
- Duration: 2011-2013
- Project coordinator: Wolfgang Wenzel
- Project leader from the University of Patras: V.G. Mavrantzas

MEKKA

- National project (synergasia) titled: *Development of carbon nanotube based polymeric membranes for industrial wastewater treatment and water reuse*
- Duration: 2011-2013
- Project coordinator: V.G. Mavrantzas

ARISTEIA 2011

- National project (Aristeia 2011) titled: *General method for the simulation of self-organization in nanostructured polymeric systems*
- Duration: 2012-2015
- Project coordinator: V.G. Mavrantzas

BioSmartTrainee

- EC research project (H2020-MSCA-ITN-2014) titled: *Training in Bio-Inspired Design of Smart Adhesive Materials (BioSmartTrainee)*
- Duration: 2015-2018
- Project coordinator: Alla Synytska (LIFP-Dresden)
- Project leader from UPatras: V.G. Mavrantzas

Limmat

- Limmat Foundation donation project (MuSiComPS) titled: *Multiscale Simulations of Complex Polymer Systems (MuSiComPS)*
- Duration: 2015-2017

- Project coordinator: D.N. Theodorou
- Project leaders from UPatras: V.G. Mavrantzas, J. Tsamopoulos

Publications in international refereed journals

1. **D.G. Tsalikis**, N. Lempesis, G. Boulougouris, D.N. Theodorou, “*On the Role of Inherent Structures in Glass-Forming Materials: I. The vitrification process*”, Journal of Physical Chemistry B, 2008, 112(34), 10619-10627.
2. **D.G. Tsalikis**, N. Lempesis, G. Boulougouris, D.N. Theodorou, “*On the Role of Inherent Structures in Glass-Forming Materials: II. Reconstruction of the Mean Square Displacement by Rigorous Lifting of the Inherent Structure Dynamics*”, Journal of Physical Chemistry B, 2008, 112(34), 10628-10637.
3. **D.G. Tsalikis**, N. Lempesis, G. Boulougouris, D.N. Theodorou, “*Efficient parallel decomposition of dynamical sampling in glass-forming materials based on an “on the fly” definition of metabasins*”, Journal of Chemical Theory and Computation, 6 (4), 1307–1322, 2010.
4. **D.G. Tsalikis**, N. Lempesis, G. Boulougouris, D.N. Theodorou, “*Temperature Accelerated Dynamics in Glass-Forming Materials*”, Journal of Physical Chemistry B, 114 (23), 7844–7853, 2010.
5. N. Lempesis, **D.G. Tsalikis**, G. Boulougouris, D.N. Theodorou, “*Lumping analysis for the prediction of long-time dynamics: from monomolecular reaction systems to inherent structure dynamics of glassy materials*”, Journal of Chemical Physics, 135 (20), 204507, 2011.
6. **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*”, Journal of Chemical Physics 139, 20476, 2013.
7. **D.G. Tsalikis**, T. Koukoulas, V.G. Mavrantzas, “*Dynamic, conformation and topological properties of ring-linear poly(ethylene oxide) blends from molecular dynamics simulations*”, Reactive and Functional Polymers 80, 61, 2014.
8. **D.G. Tsalikis**, V.G. Mavrantzas, “*Threading of Ring Poly(ethylene oxide) Molecules by Linear Chains in the Melt*”, ACS Macro Letters 3 (8), 763, 2014.
9. P. Mermigkis, **D.G. Tsalikis**, V.G. Mavrantzas, “*Determination of the effective diffusivity of water in a poly (methyl methacrylate) membrane containing carbon nanotubes using kinetic Monte Carlo simulations*”, Journal of Chemical Physics, 143(16) 164903, 2015.
10. **D.G. Tsalikis**, V.G. Mavrantzas, D. Vlassopoulos, “*Analysis of slow modes in ring polymers: threading controls long-time relaxation*”, ACS Macro Letters 5 (6), 755, 2016.
11. 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 8 (8), 283, 2016.
12. 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 and Simulations, DOI: 10.1002/mats.201600049, 2016.

Presentations (speaker is underlined):

1. G. Boulougouris, C. Tzoumanekas, **D.G. Tsalikis**, N. Kopsias, D.N. Theodorou, “*Energy landscape and entanglement network – based simulation schemes for understanding ageing and plasticity in polymer glasses*”, CECAM Workshop on Simulating deformed glasses and melts: From simple liquids to polymers, Lyon, France, September 12-14, 2005.
2. **D.G. Tsalikis**, G. Boulougouris, L. Peristeras, D.N. Theodorou, “*Ageing in atomistic simulations of amorphous glassy polymers*”, 6th Hellenic Polymer Society Conference (ELEP 2006), Patras, Greece, November, 2006.
3. **D.G. Tsalikis**, G. Boulougouris, L. Peristeras, D.N. Theodorou, “*Bridging time scale is amorphous glassy polymers*”, 4th International workshop on nonequilibrium thermodynamics and complex fluids, Rhodes, Greece, September 3-7, 2006.
4. **D.G. Tsalikis**, G. Boulougouris, C. Tzoumanekas, D.N. Theodorou, “*Atomistic and mesoscopic simulations of relaxation and plastic deformation in amorphous polymers*”, 13th International Conference on Deformation, Yield and Fracture of Polymers, Rolduc Abbey, Kerkrade, The Netherlands, April 10-13, 2006.

5. **D.G. Tsalikis**, G. Boulougouris, L. Peristeras, D.N. Theodorou, “*Plastic Deformation in Amorphous Polymers: A Free Energy Landscape Approach*”, AIChE Annual Meeting, San Francisco, California, USA, November 12-17, 2006.
6. G.C. Boulougouris, **D.G. Tsalikis**, L. Peristeras, D.N. Theodorou, “*Atomistic simulations of polymeric glasses over a wide time scale*”, 11th International Conference on Properties and Phase Equilibria, PPEPPD, Hersonissos, Crete, Greece, May 20-25, 2007.
7. **D.G. Tsalikis**, G. Boulougouris, L. Peristeras, D.N. Theodorou, “*Parallel programming strategies for the calculation of saddle points in multidimensional dynamical surfaces*”, 6th Panhellenic Conference on Chemical Engineering, Athens, Greece, May 31- June 2, 2007.
8. **D.G. Tsalikis**, G. Boulougouris, L. Peristeras, D.N. Theodorou, “*Computational study of dynamical properties for glassy polymers using the inherent structure representation*”, 6th Panhellenic Conference on Chemical Engineering, Athens, Greece, May 31- June 2, 2007.
9. **D.G. Tsalikis**, N. Lempeis, G. Boulougouris, D. N. Theodorou, “*On the role of inherent structures in glass-forming materials*”, AIChE Annual Meeting, Philadelphia, PA, USA, November 16-21, 2008.
10. **D.G. Tsalikis**, G. Boulougouris, L. Peristeras, D.N. Theodorou, “*The role of inherent structures in glass-forming materials*”, 7th Panhellenic Conference on Chemical Engineering, Patras, Greece, June 2009.
11. **D.G. Tsalikis**, N. Lempeis, G.C. Boulougouris, D.N. Theodorou, “*Energy Landscape–Based Study of Atomic Displacements in Glass Forming Materials*”, Diffusion Fundamentals III, Athens, Greece, August 23-26, 2009.
12. **D.G. Tsalikis**, C. Baig, V.G. Mavrantzas, E. Amanatides, D. Mataras, “*Hierarchical simulation of microcrystalline silicon thin films growth and structure*”, 14th International Conference on Plasma Surface Engineering, Garmisch-Patenkirchen, Germany, September 10-14, 2012.
13. T. Koukoulas, **D.G. Tsalikis**, P.S. Stephanou, V.G. Mavrantzas, “*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.
14. T. Koukoulas, **D.G. 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 Conference on Mechanics, Chania, Greece, May 25-27, 2013.
15. **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.
16. **D.G. Tsalikis**, T. Koukoulas, V.G. Mavrantzas, D. Vlassopoulos, “*Threading of ring poly(ethylene oxide) molecules by linear chains in the melt under equilibrium molecular dynamics simulations*”, 7th International Meeting of the Hellenic Rheology Society (HSR 2014), Heraklion, Greece, June 7-10, 2014.
17. **D.G. Tsalikis**, T. Koukoulas, V.G. Mavrantzas, D. Vlassopoulos, “*Dynamic, conformational and topological properties of ring PEO melts from molecular dynamics simulations and comparison with experimental data*”, 10th Hellenic Polymer Society Conference (ELEP 2014), Patras, Greece, December 4-6, 2014.
18. 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.
19. 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.
20. **D.G. Tsalikis**, V.G. Mavrantzas “*Threading of ring poly(ethylene oxide) molecules by linear chains or other rings in the melt: molecular dynamics simulations followed by a geometric analysis*”, 249th American Chemical Society National Meeting & Exposition, Denver, USA (2015).
21. **D.G. Tsalikis**, V.G. Mavrantzas “*Structural, conformational, dynamic and topological properties of ring poly(ethylene oxide) melts from molecular dynamics simulations and comparison with experimental data*”, 8th International Congress on Computational Mechanics (GRACM), Volos, Greece, July 12-15, 2015.

22. **D.G. Tsalikis**, V.G. Mavrantzas, “*Topological constraints in polymer rings*”, PRACE Scientific and Industrial Conference (PRACE days16), Budapest, Hungary, May 10-12, 2016
23. **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*”, XVII-th International Congress on Rheology (ICR 2016), Kyoto, Japan, August 8 - 13, 2016.
24. **D.G. Tsalikis**, V.G. Mavrantzas, “*Microscopic structure, conformation and dynamics of ring and linear polyethylene oxide melts from detailed atomistic molecular dynamics simulations: Dependence on chain length and direct comparison with experimental data*”, XVII-th International Congress on Rheology (ICR 2016), Kyoto, Japan, August 8 - 13, 2016.
25. **P.V. Alatas**, **D.G. 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.
26. **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.
27. **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.
28. **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.
29. **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*”, Material Research Society Fall Meeting and Exhibit (MRS 2016), Boston, USA, November 27-December 2, 2016.

References

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