



## Dimitrios G. Tsalikis

### Post-Doctoral Research Fellow

#### Personal Information

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| <b>Birth date:</b>       | 19 August 1980<br>Married  |
| <b>Current position:</b> | Post-doctoral research fellow, Department of Chemical Engineering, University of Patras              |
| <b>Work address:</b>     | 1 Caratheodori Street,<br>Department of Chemical Engineering,<br>University of Patras, Patras, 26504 |
| <b>Phone number:</b>     | 6947813112   |
| <b>Email:</b>            | <a href="mailto:tsalikis@chemeng.upatras.gr">tsalikis@chemeng.upatras.gr</a>                         |
| <b>Military service:</b> | Fulfilled (8/2009 - 4/2010)  |

#### Professional/Research experience

- 4/2011- present: **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).

#### Education

- 29/7/2004: Diploma in Chemical Engineering, University of Patras.
- 15/7/2009: 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

- 2018: Instructor, “*Introduction to Biomolecular modelling and Molecular dynamics in High Performance Computing*”, PRACE Training Event, GRNET, Athens (with Dr. Zoe Cournia and Dr. Dimitris Dellis).
- 2017-20: Instructor, course “*Rheology of Polymers*”, Interdisciplinary Graduate Program of Studies, “*Polymer Science and Technology*”, University of Patras (with Prof. V.G. Mavrantzas).
- 2016-17: Instructor, course “*Rheology of Polymers*”, Interdisciplinary Graduate Program of Studies, “*Polymer Science and Technology*”, University of Patras (with Prof. C. Tsitsilianis).
- 2014-15 Instructor, course: “*Rheology of Polymers*”, Interdisciplinary Graduate Program of Studies, “*Polymer Science and Technology*”, University of Patras (with Prof. G. Bokias).
- 2005-2009: Teaching Assistant, “*Laboratory of Physical Chemistry*”, School of Chemical Engineering NTUA.

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

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

## Awards, Honors, Fellowships

- *Best Poster Award*, 12th Hellenic Polymer Society International Conference POLYCONF12, Ioannina, Greece (2018).
- *Best Poster Award*, 11<sup>th</sup> Hellenic Polymer Society International Conference POLYCONF11, Heraklion, Greece (2016).
- *Best Poster Award*, 2<sup>nd</sup> 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).

## 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, 10619.
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, 10628.
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* **2010**, 6, 1307.
4. **D.G. Tsalikis**, N. Lempesis, G. Boulougouris, D.N. Theodorou, "Temperature Accelerated Dynamics in Glass-Forming Materials", *Journal of Physical Chemistry B* **2010**, 114, 7844.
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* **2011**, 135, 204507.
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* **2013**, 139, 20476.
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* **2014**, 80, 61
8. **D.G. Tsalikis**, V.G. Mavrantzas, "Threading of Ring Poly(ethylene oxide) Molecules by Linear Chains in the Melt", *ACS Macro Letters* **2014**, 3, 763.

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 **2015**, 143, 164903.
10. **D.G. Tsalikis**, V.G. Mavrantzas, D. Vlassopoulos, “*Analysis of slow modes in ring polymers: threading controls long-time relaxation*”, ACS Macro Letters **2016**, 5, 755.
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 **2016**, 8, 283.
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 **2016**, 26, 1600049.
13. **D. G. Tsalikis**, T. Koukoulas, V.G. Mavrantzas, R. Pasquino, D. Vlassopoulos, W. Pyckhout-Hintzem, A. Wischniewski, M. Mockenbusch and D. Richter, “*Microscopic Structure, Conformation, and Dynamics of Ring and Linear Poly(ethylene oxide) Melts from Detailed Atomistic Molecular Dynamics Simulations: Dependence on Chain Length and Direct Comparison with Experimental Data*”, Macromolecules **2017**, 50, 2565.
14. D. G. Tsalikis, P. V. Alatas, L. D. Peristeras, V. G. Mavrantzas, “*Scaling laws for the conformation and dynamics of ring poly-mers in the crossover region around Me from detailed molecular dynamics simulations*”, ACS Macro Letters **2018**, 7, 916.
15. P.S. Stephanou, **D. G. Tsalikis**, E.N. Skountzos, V.G. Mavrantzas, “*Hierarchical modeling of polymer nanocomposites: Non-equilibrium thermodynamics modeling coupled with detailed atomistic non-equilibrium molecular dynamics simulations*”, Materials Today Proceedings **2018**, 5, 27589.
16. 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.
17. D. G. Tsalikis, V.G. Mavrantzas, “*Conformation and Dynamics of Dilute Solutions of Polymer Rings in Linear Matrices from Molecular Dynamics Simulations: Dependence on Ring Size and Matrix Chain Length and Comparison with Experimental Data*”, Macromolecules in preparation

### 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*”, 6<sup>th</sup> 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*”, 4<sup>th</sup> 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*”, 13<sup>th</sup> 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*”, 11<sup>th</sup> 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*”, 6<sup>th</sup> 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*”, 6<sup>th</sup> Panhellenic Conference on Chemical Engineering, Athens, Greece, May 31- June 2, 2007.
9. **D.G. Tsalikis**, N. Lempeisis, 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*”, 7<sup>th</sup> Panhellenic Conference on Chemical Engineering, Patras, Greece, June 2009.
11. **D.G. Tsalikis**, **N. Lempeisis**, 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*”, 14<sup>th</sup> International Conference on Plasma Surface Engineering, Garmisch-Partenkirchen, 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*”, 245<sup>th</sup> 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*”, 10<sup>th</sup> 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*”, 9<sup>th</sup> 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*”, 7<sup>th</sup> 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*”, 10<sup>th</sup> 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*”, 10<sup>th</sup> 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*”, 10<sup>th</sup> 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*”, 249<sup>th</sup> 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*”, 8<sup>th</sup> 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), Prague, Czech Republic, 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*”, 2<sup>nd</sup> 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*”, 11<sup>th</sup> 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.
  30. 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*”, Annual European Rheology Conference (AERC 2017), Copenhagen, Denmark, 3-6 April 2017.
  31. P.S. Stephanou, **D.G. Tsalikis**, P.V. Alatas, V.G. Mavrantzas, “*Non-Equilibrium Thermodynamics Modelling and Atomistic Simulation of the Rheology of Unentangled Polymer Nanocomposites*” Eurofillers Polymer Blends 2017, Hersonissos, Heraklion Crete, 23-27 April 2017.
  32. **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*”, PRACEDays 2017, Barcelona Spain, 15-19 May 2017.
  33. P.V. Alatas, **D.G. Tsalikis**, V.G. Mavrantzas, “*Scaling laws for the conformation and dynamics of ring polymers in the crossover region from Rouse to non-Rouse from detailed molecular dynamics simulations*” 11th Pan-Hellenic Conference on Chemical Engineering, Thessaloniki, Greece, 25-27 May, 2017.
  34. E.N. Skountzos, **D.G. Tsalikis**, V.G. Mavrantzas, “*On the role of the end-functional groups on the microscopic structure, dynamics and chain relaxation of polymer nanocomposites*”, 11th Pan-Hellenic Conference on Chemical Engineering, Thessaloniki, Greece, 25-27 May, 2017.
  35. D. G. Mallios, **D. G. Tsalikis**, V. G. Mavrantzas, “*The Molecular Dynamics of fully atomistic detail as a studying tool of self-assembly peptide amphiphiles in characteristic nanostructures*”, 3rd Workshop of Graduates and Post-Docs in Chemical Engineering Sciences CES-WGP3, Patras, Greece, 3-4 October 2017
  36. T. S. Alexiou, **D. G. Tsalikis**, V. G. Mavrantzas, “*Atomistic Molecular Dynamics simulations of aqueous solutions of DNA molecules*”, 3rd Workshop of Graduates and Post-Docs in Chemical Engineering Sciences CES-WGP3, Patras, Greece, 3-4 October 2017.
  37. **D. G. Tsalikis**, L. D. Per T. S. Alexiou, **D. G. Tsalikis**, V. G. Mavrantzas, “*Atomistic Molecular Dynamics simulations of aqueous solutions of DNA molecules*”, 3rd Workshop of Graduates and Post-Docs in Chemical Engineering Sciences CES-WGP3, Patras, Greece, 3-4 October 2017.
  38. **D. G. Tsalikis**, L. D. Peristeras, V. G. Mavrantzas, “*Melt rheology of ring poly(ethylene oxide) melts and comparison with experimental data*”, The Annual European Rheology Conference, Sorrento, Italy, 16-19 April 2018.
  39. P.S. Stephanou, **D.G. Tsalikis**, E.N. Skountzos, V.G. Mavrantzas, “*Hierarchical modeling of polymer nanocomposites: Non-equilibrium thermodynamics modeling coupled with detailed atomistic non-equilibrium molecular dynamics simulations*”, International Workshop on Nonequilibrium Thermodynamics, Sint-Michielsgestel, The Netherlands, 1-6 July 2018.
  40. T. 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*”, 12<sup>th</sup> Hellenic Polymer Society International Conference, Ioannina, Greece, 1-3 October 2018.
  41. **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*”, 12<sup>th</sup> Hellenic Polymer Society International Conference, Ioannina, Greece, 1-3 October 2018.
42. 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*”, The Annual European Rheology Conference, Portoroz, Slovenia, 8-11 April 2019.
  43. **D. G. Tsalikis**, T. Alexiou, P. V. Alatas, V. G. Mavrantzas, “*Shear rheology of polymer melts and nanocomposites via nonequilibrium molecular dynamics simulations*”, European HPC Summit Week (PRACEdays 2019), Poznan, Poland, 13-17 May 2019.
  44. **D. G. Tsalikis**, E. N. Skountzos, P. Stephanou, V. G. Mavrantzas, “*Coupling atomistic simulations and theoretical modeling to elucidate the role of chain end-functional groups on the dynamics of polymer nanocomposites*”, European HPC Summit Week (PRACEdays 2019), Poznan, Poland, 13-17 May 2019.
  45. **D. G. Tsalikis**, T. Alexiou, P. V. Alatas, V. G. Mavrantzas, “*The role of chain end-functional groups on microstructure and microdynamics of polymer nanocomposites*”, 12<sup>th</sup> Panhellenic Conference on Chemical Engineering, Greece, 29-31 May 2019.
  46. **D. G. Tsalikis**, T. Alexiou, P. V. Alatas, V. G. Mavrantzas, “*Shear rheology of marginally entangled ring polymer melts through non-equilibrium atomistic molecular dynamics simulations*”, European Polymer Congress 2019, Heraklion, Greece, 9-13 June 2019.
  47. **D. G. Tsalikis**, A. J. Tsamopoulos, A. F. Katsarou, V. G. Mavrantzas, “*Steady shear flow of marginally entangled ring polymer melts through nonequilibrium molecular dynamics simulations*”, 9<sup>th</sup> International Conference of the Hellenic Society of Rheology, 2019, Samos, Greece, 23-27 June 2019.

## Invited talks

1. **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*”, Workshop on Algebraic modeling of topological and computational structures at NTUA, Athens, Greece 1-3 July 2015.
2. **D. G. Tsalikis**, V. G. Mavrantzas, “*Microscopic structure, conformational, dynamical and topological properties of ring polyethylene oxide (PEO) melts from detailed atomistic molecular dynamics simulations: Dependence on chain length and direct comparison with experimental data*”, Workshop on Mathematical and Computational Techniques for Molecular Systems at FORTH, University of Crete - ACMAC, Heraklion, Greece, September 2015.
3. **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*”, Focused Workshop on Ring Polymers, Heraklion, Greece, 25-27 September 2017.
4. **D. G. Tsalikis** “*Extending a Commercial Simulation Engine to Conduct Rigorously Atomistic Simulations Under Flow: Application to Polymers Melts of Various Molecular Architectures and Polymer Nanocomposite Materials*”, Focused Workshop on the Multiscale Modelling of Polymer Matrix Nanocomposite Materials, Nicosia, Cyprus, 3 May 2018.
5. **D. G. Tsalikis** “*High Performance Computing and Atomistic Simulations of Polymeric Materials*”, Digital Technology Symposium, Athens, Greece, 5-6 November 2018.

## Research Projects

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| <p><b>MMM@HPC</b></p> <ul style="list-style-type: none"> <li>• EC (FP7-INFRA-2010-1.2.2) project titled: <i>Multiscale materials modeling on high performance computing (MMM@HPC)</i></li> <li>• Duration: 2011-2013</li> </ul> | <p><b>MEKKA</b></p> <ul style="list-style-type: none"> <li>• National project (synergasia) titled: <i>Development of carbon nanotube based polymeric membranes for industrial wastewater treatment and water reuse</i></li> <li>• Duration: 2011-2013</li> </ul> | <p><b>ARISTEIA 2011</b></p> <ul style="list-style-type: none"> <li>• National project (Aristeia 2011) titled: <i>General method for the simulation of self-organization in nanostructured polymeric systems</i></li> <li>• Duration: 2012-2015</li> </ul> |
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- Project coordinator: W. Wenzel
- Project coordinator: V.G. Mavrantzas
- 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)

#### **EDBM 34**

- Supporting researchers with emphasis given in young researchers (MIS 5004866): *Conformational and transport properties of cyclic biological and synthetic polymer solutions: theory and atomistic simulation*
- Duration: 2018-2019
- Project coordinator: V.G. Mavrantzas
- Researchers: **D. G. Tsalikis**, T. S. Alexiou, P. V. Alatas

#### **MuSiComPS**

- Limmat Foundation donation project titled: *Multiscale Simulations of Complex Polymer Systems (MuSiComPS)*
- Duration: 2015-2018
- Project coordinator: D.N. Theodorou

#### **FORTH SYNERGY GRANT**

- Titled: *"Shear and planar elongational rheology of entangled ring melts"*
- Duration: 2019-2021
- Project coordinators: D. Vlassopoulos and V.G. Mavrantzas

#### **FORCE**

- EC research project (H2020-NMBP-2016-2017) titled: *Formulations and Computational Engineering (FORCE)*
- Duration: 2016-2020
- Project coordinator: Adham Hashibon (Fraunhofer IWM/ITWM)

## Professional activities

- Reviewer for *Soft Matter* (Royal Society of Chemistry), *Plasma Process and Polymers* (Wiley), *International Journal of Modern Physics* (WorldScientific), *Journal of Chemical Information and Modeling* (American Chemical Society), *Polymers* (MDPI)
- Reviewer Board: *Polymers* (MDPI)
- American Chemical Society, regular fellow
- European Society of Rheology
- Hellenic Society of Rheology
- PRACE Expert
- Technical Chamber of Greece

## References

Prof. Vlasios G. Mavrantzas  
 Department of Chemical Engineering  
 University of Patras, GR 26504, Greece  
 &  
 Dept. of Mechanical & Process Engineering  
 ETH-Zurich, CH-8092, Switzerland  
 e-mail: [vlasios@chemeng.upatras.gr](mailto:vlasios@chemeng.upatras.gr)  
 tel.: +30-6944-602580

Prof. Doros Theodorou  
 Department of Chemical Engineering  
 National Technical University of Athens  
 9 Heron Polytechniou St., Zographou, Athens,  
 Greece GR 157 80  
 e-mail: [doros@chemeng.ntua.gr](mailto:doros@chemeng.ntua.gr)  
 tel.: +30 210 772 3157

Prof. Sachin Shanbhag  
 Department of Scientific Computing  
 Florida State University

Prof. Dimitris Vlassopoulos  
 Department of Materials Science  
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