# Prof. Vagelis A. Harmandaris

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## Education

Ph.D. in Chemical Engineering
University of Patras, Greece, February 2002
- *GPA*: Highest degree
- *Dissertation*: "Atomistic Molecular Dynamics Simulations of Polymer Melt Viscoelasticity"
- *Advisor*: Prof. D.N. Theodorou

Diploma in Chemical Engineering
University of Patras, Greece, July 1996

## Professional Experience

Associate Professor (March 2016 - Today)
Department of Mathematics and Applied Mathematics, University of Crete, Greece

Tenured Assistant Professor (December 2014 – March 2016)
Department of Applied Mathematics, University of Crete, Greece

Track Tenure Assistant Professor (September 2009 – December 2014)
Department of Applied Mathematics, University of Crete, Greece

Visiting Scientist
(January 2010 – Today)
Max Planck Institute for Polymer Research (MPIP), Theory Group, Mainz, Germany

Research Associate
(October 2007 – August 2009)
Max Planck Institute for Polymer Research (MPIP), Theory Group, Mainz, Germany

Post-Doctoral Research Associate
(February 2005 – September 2007)
Max Planck Institute for Polymer Research (MPIP), Theory Group, Mainz, Germany
(May 2003 – January 2005)
Institute of Chemical Engineering and High-Temperature Chemical Processes and Department of Chemical Engineering, University of Patras, Patras, Greece

Ph.D. Research Assistant (September 1996-November 2001)
Department of Chemical Engineering, University of Patras, Greece, and
Institute of Chemical Engineering and High-Temperature Chemical Process (ICE/HT-FORTH)

## Honors and Awards

- Chairman, co-chairman or co-organizer of 3 international scientific conferences and workshops.
- Who's Who in Science 2008, 2010 Edition.
- European fellowship Marie-Curie for participating in the «*International School of Solid State Physics: 34th Course: Computer Simulations in Condensed Matter*», Erice, Italy, 2005.
- Ph.D. Research assistant fellowship, Institute of Chemical Engineering and High-Temperature Chemical Process (ICE/HT-FORTH), 1996-2001.
- European fellowship for participating as a training visitor in University of Edinburgh under the program TRACS, UK, 2000.
- Outstanding Undergraduate Student Excellence Awards, 1993 and 1994.

## Professional Affiliations

Member, Society of Industrial and Applied Mathematics (SIAM), American Chemical Society (ACS), American Physical Society (APS), Hellenic Society of Rheology (HSR), Polymer Hellenic Society, Technical Camber of Greece (TEE).

### Referee / Organizer

- For about *30 international journals* among which: Nature Materials, Nature Communications, Physical Review Letters, Macromolecules, Journal of the American Chemical Society, Soft Matter, The Journal of Chemical Physics, Physical Review E, Physical Chemistry Chemical Physics, Langmuir, Journal of Polymer Science Part B, Journal of Physical Chemistry, Macrom. Theory and Simulation, Rheologica Acta, Polymer, etc.
- *Reviewer for:* European Commission; National Science Foundation (NSF), USA; Deutschen Forschungsgemeinschaft (DFG), Germany; General Secretariat for Research and Technology (GSRT), Greece; State Scholarships Foundation (IKY), Greece; Swiss National Science Foundation (SNSF), Switzerland; Israel National Science Foundation (INSF), Israel; Romanian National Research Council; Partnership for Advanced Computing in Europe (PRACE) Expert, Europe.
- *Organizer*: Member of the organizing and/or scientific committee for 10 international and national conferences and workshops, among which: (1) The International Conference "Eurofillers Polymer Blends", Heraklion, Crete, April 23-27, 2017; (2) SIAM 2016, Minisymposium on "Numerical Methods on Multiscale Materials Modeling", Philadelphia, May 8-12, 2016.

## Publications in Refereed Journals

1. A. F. Behbahani, S.M. Vaez Allaei, G.H. Motlagh, H. Eslami and **V. Harmandaris**, "Structure and dynamics of stereo-regular poly(methyl-methacrylate) melts through atomistic molecular dynamics simulations", *Soft Matter*, **2018**, *14*, 1449-1464, doi: 10.1039/C7SM02008B. https://doi.org/10.1039/C7SM02008B

2. A. Tsourtis, **V. Harmandaris**, D. Tsagkarogiannis, "Parameterization of Coarse-grained Molecular Interactions through Potential of Mean Force Calculations and Cluster Expansions Techniques", *Entropy*, **2017**, *19*, 395, doi:10.3390/e19080395.

3. A. Rissanou, H. Papananou, V. Petrakis, M. Doxastakis, K. Andrikopoulos, G. Voyiatzis, K. Chrissopoulou, **V. Harmandaris**, S. Anastasiadis, "Structural and Conformational Properties of Poly(ethylene oxide)/Silica Nanocomposites: Effect of Confinement", *Macromolecules*, **2017**, *50*, 6273-6284; Doi:10.1021/acs.macromol.7b00811. http://dx.doi.org/10.1021/acs.macromol.7b00811

4. M. Gulde, A. Rissanou, **V. Harmandaris**, M. Müller, S. Schäfer, C. Ropers "Structure and dynamics of monolayer polymer crystallites on graphene", *Nano Letters*, **2016**, *16*, 6994–7000; doi:10.1021/acs.nanolett.6b03079, http://pubs.acs.org/doi/abs/10.1021/acs.nanolett.6b03079

5. E. Kalligiannaki, A. Chazirakis, A. Tsourtis, M. Katsoulakis, P. Plechac, **V. Harmandaris**, "Parametrizing

coarse grained models for molecular systems at equilibrium", *Europ. Phys. J. Special Topics*, **2016**, *225*, 1347–1372. doi: 10.1140/epjst/e2016-60145-x. http://link.springer.com/article/10.1140/epjst/e2016-60145-x

6. **V. Harmandaris**, E. Kalligiannaki, M. Katsoulakis, P. Plechac, "Path-space variational inference for non-equilibrium coarse-grained systems", *J. Comp. Phys.*, **2016**, *314*, 355–383. http://www.sciencedirect.com/science/article/pii/S002199911600173X

7. P. Bačová, A. Rissanou, **V. Harmandaris**, "Edge-functionalized Graphene as a nanofiller: Molecular Dynamics Simulation Study", *Macromolecules*, **2015**, *48*, 9024–9038, http://pubs.acs.org/doi/10.1021/acs.macromol.5b01782.

8. E. Kalligiannaki, **V. Harmandaris**, M. Katsoulakis, P. Plechac "The geometry of generalized force matching and related information metrics in coarse-graining of molecular systems", *J. Chem. Phys.*, **2015**, *143*, 084105. http://dx.doi.org/10.1063/1.4928857

9. A. Tsourtis, Y. Pantazis, M. Katsoulakis, **V. Harmandaris**, "Parametric Sensitivity Analysis for Stochastic Molecular Systems using Information Theoretic Metrics", *J. Chem. Phys.*, **2015**, *143*, 014116.

10. A. Rissanou, **V. Harmandaris**, "Structural and Dynamical Properties of Polystyrene Thin Films", *Macromolecules*, **2015**, *48*, 2761–2772.

11. A. Rissanou, A. Power, **V. Harmandaris**, "Properties of Polyethylene/Graphene Nanocomposites through Molecular Dynamics Simulations", *Polymers*, **2015**, *7*, 390-417; doi:10.3390/polym7030390.

12. H. J. Butt, H. Duran, W. Egger, F. Faupel, **V. Harmandaris**, S. Harms, K. Johnston, K. Kremer, Y. Lin, L. Lue, C. Ohrt, K. Raetzke, L. Ravelli, W. Steffen, and S. D. B. Vianna, "Interphase of a polymer at a solid interface", *Macromolecules*, **2014,** *47*, 8459-8465.

13. **V. Harmandaris**, "Quantitative study of equilibrium and non-equilibrium polymer dynamics through systematic hierarchical coarse-graining simulations", *Korea-Aust. Rheol. J.*, **2014**, *26*, 15-28.

14. A. Rissanou, **V. Harmandaris**, "Dynamics of various polymer/graphene interfacial systems through atomistic molecular dynamics simulations", *Soft Matter*, **2014**, in press, DOI: 10.1039/C3SM52688G.

15. K. Johnston, **V. Harmandaris**, "Hierarchical multiscale modeling of polymer−solid interfaces: Atomistic to coarse-grained description and structural and conformational properties of polystyrene−gold systems", *Macromolecules*, **2013,** *46*, 5741−5750.

16. **V. Harmandaris**, M. Doxastakis "Molecular dynamics of polyisoprene/polystyrene oligomer blends: The role of self-concentration and fluctuations on blend dynamics", *J. Chem. Phys.*, **2013,** *139*, 034904.

17. A. Rissanou, **V. Harmandaris**, "A molecular dynamics study of polymer/graphene nanocomposites", *Macromolecular Symposia*, **2013**, *331-332*, 43–49.

18. K. Johnston, **V. Harmandaris**, "Hierarchical simulations of hybrid polymer/solid materials", *Soft Matter*, **2013**, *9*, 6696-6710 (Review article, Themed Issue on Emerging Investigators).

19. **V. Harmandaris**, G. Floudas, K. Kremer, "Dynamic heterogeneity in fully miscible blends of polystyrene with oligostyrene", *Phys. Rev. Let.* **2013**, *110*, 165701.

20. A. Rissanou, **V. Harmandaris**, "Structure and dynamics of poly(methyl-methacrylate)/graphene systems through Atomistic molecular dynamics Simulations", *Journal of Nanoparticle Research* **2013**, 15, 1589.

21. A. Rissanou, E. Georgilis, M. Kasotaskis, A. Mitraki, **V. Harmandaris**, "Effect of solvent on the self-assembly of dialanine and diphenylalanine peptides", *J. Phys. Chem. B* **2013**, *117*, 3962-3975.

22. K. Johnson, **V. Harmandaris**, "Properties of short polystyrene chains confined between two gold surfaces through a combined density functional theory and classical molecular dynamics approach",

*Soft Matter*, **2012,** *8*, 6320-6332.

23. K. Johnson, **V. Harmandaris**, "Properties of benzene confined between two Au(111) surfaces using a combined density functional theory and classical molecular dynamics approach.", *J. Phys. Chem. C* **2011**, *115*, 14707-14717.
24. D. Fritz, K. Koschke, **V. Harmandaris**, N.F.A. van der Vegt and K. Kremer, "Multiscale modeling of soft matter: scaling of dynamics", *Phys. Chem. Chem. Phys.,* **2011**, *13*, 10412-10420.
25. **V. Harmandaris**, G. Floudas, K. Kremer, "Temperature and pressure dependence of polystyrene dynamics through molecular dynamics simulations and experiments", *Macromolecules* **2011**, *44*, 393-402.
26. C. Baig, **V. Harmandaris** "Quantitative Analysis on the Validity of a Coarse-Grained Model for Nonequilibrium Polymeric Liquids under Flow", *Macromolecules*, **2010**, *43*, 3156-3160.
27. D. Fritz, **V. Harmandaris**, K. Kremer, N. van der Vegt, "Coarse-Grained polymer melts based on isolated atomistic chains: Simulation of polystyrene of different tacticities, *Macromolecules*, **2009**, *42*, 7579-7588.
28. **V. Harmandaris**, K. Kremer, "Predicting polymer dynamics at multiple length and time scales", *Soft Matter*, **2009**, *5*, 3920-3926.
29. T. Cherdhirankorn, **V. Harmandaris**, A. Juhari, P. Voudouris, G. Fytas, K. Kremer, K. Koynov, "Fluorescence correlation spectroscopy study of molecular probe diffusion in polymer melts", *Macromolecules* **2009**, *42*, 4858-4866.
30. **V. Harmandaris**, K. Kremer, "Dynamics of polystyrene melts through hierarchical multiscale simulations", *Macromolecules*, **2009**, *42*, 791-802.
31. T. Mulder, **V. Harmandaris**, A.V. Lyulin, N.F.A. van der Vegt, K. Kremer, M.A.J. Michels, "Structural properties of atactic polystyrene of different thermal history obtained from a multi-scale simulation", *Macromolecules*, **2009**, *42*, 384-391.
32. T. Mulder, **V. Harmandaris**, A.V. Lyulin, N.F.A. van der Vegt, M.A.J. Michels, "Molecular simulation via connectivity-altering Monte Carlo and Scale-jumping methods: Application to amorphous polystyrene", *Macrom. Theory Simul.*, **2008**, *17*, 393-402.
33. T. Mulder, **V. Harmandaris**, A.V. Lyulin, N.F.A. van der Vegt, B. Vorselaars, M.A.J. Michels, "Equilibration and deformation of amorphous polystyrene: Scale-jumping simulation approach", *Macrom. Theory Simul.*, **2008**, *17*, 290-300.
34. G. Tsolou, **V. Harmandaris**, V.G. Mavrantzas, "Molecular dynamics simulation of temperature and pressure effects on the intermediate length scale dynamics and zero shear rate viscosity of cis-1,4-polybutadiene: Rouse mode analysis and dynamic structure factor spectra", *J. Non-Newt. Fl. Mech.*, **2008**, *152*, 184.
35. **V. Harmandaris**, D. Reith, N.F.A. van der Vegt, K. Kremer, "Comparison between coarse-graining models for polymer systems: Two mapping schemes for polystyrene", *Macrom. Chem. and Phys.*, **2007**, 2*08*, 2109.
36. **V. Harmandaris**, N. Adhikari, N.F.A. van der Vegt, K. Kremer, R.Voelkel, C.C. Liew, H. Weiss, "Ethylbenzene diffusion in polystyrene: United atom atomistic/coarse grained simulations and experiments", *Macromolecules*, **2007**, *40*, 7026.
37. B. Reynolds, G. Illya, **V. Harmandaris**, M.M. Müller, K. Kremer, M. Deserno, "Mediated interactions between colloids adsorbed on a biological membrane", *Nature*, **2007**, *447*, 461. Also in News and Views, Nature **2007**,*447*, 387. Also featured in the Virtual Journal of Biological Physics Research, June 1, 2007 issue.
38. O. Alexiadis, **V. Harmandaris**, V. Mavrantzas, L. de la Sitte, "Atomistic simulation of alkanethiol self-assembled monolayers on different metal surfaces via a quantum first-principles parameterization of the sulfur-metal interaction", *J. Phys. Chem. C*, **2007**, *111*, 6380.

39. **V. Harmandaris**, M. Deserno, "A novel method for measuring the bending rigidity of model lipid membranes by simulating tethers", *J. Chem. Phys*., **2006**, *125*, 204905. Also featured in the Virtual Journal of Biological Physics Research, December 1, 2006 issue.

40. **V. Harmandaris**, N. Adhikari, N.F.A. van der Vegt, K. Kremer "Hierarchical modeling of polystyrene: From atomistic to coarse-grained simulations", *Macromolecules*, **2006**, *39*, 6708.

41. G. Tsolou, **V. Harmandaris**, V.G. Mavrantzas, "Temperature and pressure effects on local structure and chain packing in cis-1,4-polybutadiene from detailed molecular dynamics simulations", *Macrom. Theory Simul*. **2006**, *15*, 381.

42. G. Tsolou, **V. Harmandaris**, V.G. Mavrantzas, "Atomistic molecular dynamics simulation of the temperature and pressure dependences of local and terminal relaxations in cis-1,4-polybutadiene", *J. Chem. Phys*., **2006**, *124*, 084906.

43. C. Baig, B.J. Edwards, D.J. Keffer, H.D. Cochran, **V. Harmandaris** "Rheological and structural studies of linear polyethylene melts under planar elongational flow using nonequilibrium molecular dynamics simulations", *J. Chem. Phys*., **2006**, *124*, 084902.

44. K. Daoulas, D.N. Theodorou, **V. Harmandaris**, N.G. Karayiannis, V.G. Mavrantzas, "Self-consistent field study of compressible semiflexible melts adsorbed on a solid substrate and comparison with atomistic simulations", *Macromolecules*, **2005**, *38*, 7134-7149.

45. **V. Harmandaris**, K. Daoulas, V.G. Mavrantzas, "Molecular dynamics simulation of a polymer melt/solid interface: Local dynamics and chain mobility in a thin film of polyethylene melt adsorbed on graphite", *Macromolecules*, **2005**, *38*, 5796-5809.

46. K. Daoulas, **V. Harmandaris**, V.G. Mavrantzas, "Detailed atomistic simulation of a polymer melt / solid interface: Structure, density and conformation of a thin polyethylene melt film adsorbed on graphite", *Macromolecules*, **2005**, *38*, 5780-5795.

47. **V. Harmandaris**, V.G. Mavrantzas, D.N. Theodorou, M. Kröger, J. Ramírez, H.C. Öttinger, D. Vlassopoulos, "Dynamic crossover from Rouse to entangled polymer melt regime: Signals from long, detailed atomistic molecular dynamics simulations, supported by rheological experiments", *Macromolecules*, **2003**, *36*, 1376-1387.

48. **V. Harmandaris**, D. Angelopoulou, V.G. Mavrantzas, D.N. Theodorou, "Atomistic molecular dynamics simulation of diffusion in binary n-alkane/polyethylene melts", *J. Chem. Phys*., **2002**, *116*, 7656-7665.

49. **V. Harmandaris**, M. Doxastakis, V.G. Mavrantzas, D.N. Theodorou, "Detailed molecular dynamics simulation of the self-diffusion of n-alkane and cis-1,4 polyisoprene oligomer melts", *J. Chem. Phys*., **2002**, *116*, 436-446.

50. **V. Harmandaris**, V.G. Mavrantzas, D.N. Theodorou, "Atomistic molecular dynamics simulations of stress relaxation upon cessation of steady-state uniaxial elongational flow", *Macromolecules*, **2000**, *33*, 8062-8076.

51. **V. Harmandaris**, V.G. Mavrantzas, D.N. Theodorou, "Atomistic molecular dynamics simulations of polydisperse linear polyethylene melts", *Macromolecules*, **1998**, *31*, 7934-7943.

## Publications Submitted or in Preparation

52. A. Tsourtis, **V. Harmandaris**, D. Tsagkarogiannis, "Parameterization of Coarse-grained Molecular Interactions through Potential of Mean Force Calculations and Cluster Expansions Techniques", submitted to *J. Chem. Phys.*

53. A. Rissanou, P. Bačová, **V. Harmandaris**, "Dynamics and wrinkling of Graphene in graphene bed polymer nanocomposites through molecular dynamics simulations", to be submitted.

54. G. Zhang, A. Xazirakis, **V. Harmandaris**, T. Stuehn, K. Daoulas, K. Kremer, "Hierarchical modeling of

polystyrene melts: from soft blobs to atomistic resolution", to be submitted.

55. V. Petrakis, A. Rissanou, **V. Harmandaris**, k. Chrissopoulou, S. Anastasiadis, "Structural properties of Polymer/Silica nanocomposites through experiments and molecular simulations", under preparation.

**Books and Chapter in Books**

1. S. Komineas, **V. Harmandaris**, "Mathematical Modelling", (in Greek) e-Textbook, *Hellenic Academic E-Books – Kallipos*, Greece, **2016.**
2. **V. Harmandaris,** M. Katsoulakis, "Computational and mathematical hierarchical modeling of molecular systems", **in preparation, 2013.**
3. **V. Harmandaris,** V.G. Mavrantzas, "Atomistic Molecular Dynamics Simulation of Segmental Dynamics in Molten Polyethylene and Comparison with Experimental Data", Chapter in Book "Recent Research Topics and Developments in Chemical Physics: From Nanoscale to Macroscale", Edited by A.F. Terzis and E. Paspalakis, Research Signpost, India, **2009.**
4. **V. Harmandaris,** V.G. Mavrantzas, "Molecular Dynamics Simulations of Polymers", Chapter in Book "Simulation Methods for Polymers", Edited by M.J. Kotelyanskii and D.N. Theodorou, Marcel Dekker, New York, **2004.**

**About 60 Publications in Peer-Reviewed Conferences and Conference Proceedings.**

**About 100 Presentations in International Conferences and Invited Presentations.**

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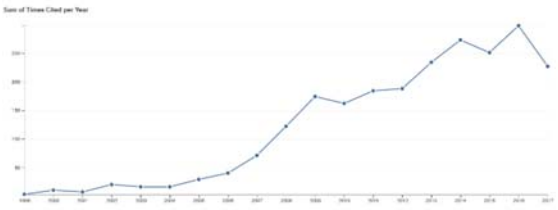

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