

## Curriculum vitae

- *Name* : Karatasos Kostas
- *Year of Birth* : 1969
- *Professional Status* : Professor at the Chemical Engineering Department, Aristotle University of Thessaloniki, Greece
- *Institutional Address* :  
University of Thessaloniki,  
Department of Chemical Engineering  
Section of Chemistry, Physical Chemistry Lab  
P.O BOX 420, 54124 Thessaloniki, Greece
- *Nationality* : Greek
- *University graduation date* :1991
- *Background* : B.S in Physics (first honours degree, National Scholarship for Excellency) , MSc in Physical Chemistry (first honours degree), PhD in Polymer Science (first honours degree, Research Scholarship, Foundation for Research and Technology Hellas – FORTH))
- *Institute of Graduation* : University of Crete, Heraklion Crete, Greece
- *Brief CV since Graduation* : Un. Of Crete, M.Sc. in Physical Chemistry 1993, Un. Of Crete, Chemistry Dept. Ph.D. 1997, Dec1997-Feb2000 Post Doctoral Fellow, University of Leeds, UK, March 2000-June 2001 Post Doctoral Fellow at Libre Universite Brussels , Belgium August 2001 – August 2002 military service September 2002-February 2003 Visiting Professor, Materials Science and Engineering Department, University of Crete. March 2003- April 2008, Lecturer at Aristotle University of Thessaloniki, Chemical Engineering Department, April 2008 – July 2014, Assistant Professor (tenure November 2011), July 2014- February 2020, Associate Professor at Aristotle University of Thessaloniki, Chemical Engineering Department, March 2020-now, Professor at Aristotle University of Thessaloniki, Chemical Engineering Department, Sabbatical leave, February 2010 – June 2010 (Molecular Simulation Engineering Laboratory, Department of Materials and Natural Resources, University of Trieste, Italy), Sabbatical leave (September 2017-August 2018), Foundation for Research and Technology – Hellas (FO.R.T.H)

## Areas of interest

- Statics, Dynamics and Thermodynamics of polymeric materials
- Molecular recognition and self-assembly in soft matter
- Glass transition and critical phenomena in soft matter
- Polymer-based Composite materials
- Biopharmaceutical applications of polymers

## Teaching/Student supervision

### Teaching

Physical Chemistry (University of Crete, Chemistry Dept. Visting Professor)  
Introduction to computer science (University of Crete, Materials Science and Technology Dept., Visiting Professor)

Physical Chemistry Labs (University of Thessaloniki, Chem. Engineering Dept.)  
Thermodynamics and Kinetics of Materials (Univ. of Thessaloniki, MSc. Course in “Advanced Materials” post graduate programme)

Computational Materials Science (Univ. of Thessaloniki, Chem. Engineering Dept.)

Nanotechnology and Soft Matter (Univ. of Thessaloniki, Chem. Engineering Dept.)

Nanostructures and physical chemistry of soft matter (Univ. of Thessaloniki, Chem. Engineering Dept., post graduate)

Physical chemistry of molecular and macromolecular systems (Univ. of Thessaloniki, Chem. Engineering Dept., post graduate)

Physical Chemistry I (Univ. of Thessaloniki, Chem. Engineering Dept.)

Science and Technology of Polymers (Univ. of Thessaloniki, Chem. Engineering Dept.)

Applied Thermodynamics matter (Univ. of Thessaloniki, Chem. Engineering Dept., post graduate)

Modeling and Simulation of Molecular Systems (Univ. of Thessaloniki, Chem. Engineering Dept., post graduate)

### **Student supervision**

4 PhDs finished (3 as principal supervisor, 1 as co-supervisor), 3 MSc finished (Single Supervisor), currently (2021) co-supervising 5 PhD Students

Participation in the examination committees of ~75 undergraduate students (diploma thesis), 9 MSc students (Master's Degree) and 29 PhD students

Supervision of 4 post-doctoral associates (currently, 2021, supervising 2)

### **Publications in refereed journals**

1. **"Coordinated X-ray and optical observation of Scorpius X-1"**  
T. Augusteijn, K. Karatasos, M. Papadakis, G. Paterakis, S. Kikuchi, N. Brosch, E. Leibowitz, P. Hertz, K. Mitsuda, T. Dotani, W.H.G Lewin, M. van der Klis, J. van Paradijs  
*Astron. & Astroph.* ,**265**, 117-182 (1992)
2. **"Local and Global Chain Dynamics in Diblock Copolymer Melts"**  
G. Fytas, S.H. Anastasiadis, K. Karatasos, and N. Hadjichristidis  
*Physica Scripta*,**T49** ,237 (1993)
3. **"Composition Fluctuation effects on Dielectric Normal Mode Relaxation in Diblock Copolymers. I Weak Segregation Regime"**  
K. Karatasos, S. H. Anastasiadis, G. Fytas, A. N. Semenov, M. Pitsikalis, and N. Hadjichristidis  
*Macromolecules* **27** ,3543 (1994)
4. **"Composition Fluctuation Effects on Dielectric Normal Mode Relaxation in Diblock Copolymers. II Disordered State in the proximity to the ODT and Ordered State"**  
K. Karatasos, S.H. Anastasiadis, G. Floudas, G. Fytas, S. Pispas, N. Hadjichristidis, T. Pakula  
*Macromolecules* ,**29**, 1326, (1996)
5. **"Computer Simulation of the Static and Dynamic Behavior of Diblock Copolymer Melts"**  
T. Pakula, K. Karatasos, S. H. Anastasiadis, G. Fytas  
*Macromolecules* , **30**, 8463 (1997)
6. **"Ordering and viscoelastic relaxation in multiarm star polymer melts"**  
D. Vlassopoulos, T. Pakula, G. Fytas, J. Roovers, K. Karatasos, N. Hadjichristidis  
*Europhysics Letters*, **39**, 617(1997)
7. **"Segmental dynamics and incompatibility in Hard/Soft Binary Polymer Blends"**  
K. Karatasos, G. Vlachos, D. Vlassopoulos, G. Fytas, G. Meier, A. Du Chesne  
*Journal of Chem. Phys.*, **108**, 5997 (1998)
8. **"Depolarized light scattering from critical polymer blends"**  
A.N. Semenov, A.E. Likhtman, D. Vlassopoulos, K. Karatasos, G. Fytas  
*Macromolecular Theory and Simulation* **8**(3), 179 (1999)

9. **"Segmental Dynamics of Miscible PI/PVE Blends: Comparison of the Predictions of a Concentration Fluctuation Model to Experiment"**  
S. Kamath, R. H. Colby, S. K. Kumar, K. Karatasos, G. Floudas, G. Fytas, J. Roovers  
*Journal of Chem. Phys.*, **111**, 6121 (1999)
10. **"On the Loops to Bridges Ratio in Ordered Triblock Copolymers: An investigation by Dielectric Relaxation Spectroscopy and Computer Simulations"**  
K. Karatasos, S. H. Anastasiadis, H. Watanabe and T. Pakula  
*Macromolecules*, **33**, 523 (2000)
11. **"Nanoscope confinement effects on local dynamics"**  
S. H. Anastasiadis, K. Karatasos, G. Vlachos, E. Manias, E. P. Giannelis  
*Phys. Rev. Lett.*, **84**(5), 915 (2000)
12. **"Effects of density on the local dynamics and conformational statistics in polyethylene: a Molecular Dynamics Study"**  
K. Karatasos, D. B. Adolf, S. Hotston  
*J. Chem. Phys.* (2000) **112**(19), 8695, (2000)
13. **"Slow modes in local polymer dynamics"**  
K. Karatasos and D. B. Adolf  
*J. Chem. Phys. (Communication)* **112**(19), 8225, (2000)
14. **"Short length-scale dynamics of Polyisobutylene by molecular dynamics simulations"**  
K. Karatasos, F. Saija and J.-P. Ryckaert  
*Physica B* **301**, 119, (2001) (corresponding author)
15. **"Polyisobutylene dynamics revisited"**  
K. Karatasos, and J.-P. Ryckaert  
*Macromolecules* **34**, 7232 (2001) (Communication) (corresponding author)
16. **"An Investigation into the local segmental dynamics of Polyethylene: an isothermal/isobaric molecular dynamics study "**  
S. Hotston, D. B. Adolf, K. Karatasos  
*J. Chem. Phys.* **115**(5), 2359, (2001)
17. **"Statics and Dynamics of model dendrimers as studied by molecular dynamics simulations"**  
K. Karatasos, D. B. Adolf and G. R. Davies  
*J. Chem. Phys.* **115**, 5310 (2001) (corresponding author)
18. **"Methyl dynamics and  $\beta$ -relaxation in polyisobutylene: comparison between experiments and molecular dynamics simulations"**  
K. Karatasos, J. -P. Ryckaert, R. Ricciardi and F. Lauprêtre  
*Macromolecules* **35**, 1451 (2002) (corresponding author)
19. **"Segmental Dynamics of Atactic Polypropylene as Revealed by Molecular Simulations and Quasielastic Neutron Scattering"**  
O. Ahumada, D. Theodorou, A. Triolo, V. Arrighi, K. Karatasos, and J.-P. Ryckaert  
*Macromolecules*, **35**, 7110 (2002)
20. **" Local Dynamics of Polyethylene and its Oligomers : A Molecular Dynamics Interpretation of the Incoherent Dynamic Structure Factor "**  
G. Arialdi, K. Karatasos, J.-P. Ryckaert, V. Arrighi , F. Saggio, A. Triolo A. Desmedt, J. Pieper, and A. E. Lechner  
*Macromolecules* **36**, 8864 (2003)
21. **"Static and dynamic behavior in model dendrimer melts: toward the glass transition"**

K. Karatasos  
*Macromolecules* **38**, 4472-4483 (2005)

**22. "Glass Transition in Dendrimers"**

K. Karatasos  
*Macromolecules* 39,4619-4626 (2006)

**23. "Segmental Dynamics under severe Connectivity Constraints: the Dendrimer Case"**

K. Karatasos, A.V. Lyulin  
*Journal of Chemical Physics* (2006) **125**, 184907 (corresponding author)

**24. "Computational polymer dynamics via DL\_POLY"**

Adolf DB, Butler SN, Drew PM, Hotston S, Karatasos K  
*MOL SIMULAT* 32 (12-13): 1017-1023 OCT-NOV 2006

**25. "Non-Gaussianity of Glassy Dynamics by Cage-to-Cage Motion"**

B. Vorselaars, A.V. Lyulin, K. Karatasos and M. A. J. Michels  
*Phys. Rev. E.*, Art. No. 011504 Part 1 JAN 2007

**26. "Effects of Topology and Size on Statics and Dynamics of Complexes of Hyperbranched Polymers with Linear Polyelectrolytes"**

G. K. Dalakoglou, K. Karatasos, S.V.Lyulin, A.V.Lyulin  
*Journal of Chemical Physics*, Art. No. 214903 (2007) (corresponding author)

**27. "Self Organization in Dendrimer Polyelectrolytes"**

K.Karatasos  
*Macromolecules* **2008**, 41, (3), 1025-1033

**28. "Structural Effects in Overcharging in Complexes of Hyperbranched Polymers with Linear Polyelectrolytes"**

S.V. Lyulin, K. Karatasos, A. Darinskii, S. Larin, and A. Lyulin  
*Soft Matter* **2008**, 4, (3), 457 (Communication)

**29. "Shear induced effects in Hyperbranched-Linear Polyelectrolyte Complexes"**

G. K. Dalakoglou, K. Karatasos, S.V.Lyulin, A.V.Lyulin  
*Journal of Chemical Physics*, 129, 034901 (2008) (corresponding author)

**30. "Brownian dynamics simulations of complexes of hyperbranched polymers with linear polyelectrolytes: Effects of the strength of electrostatic interactions on static properties"**

G. K. Dalakoglou, K. Karatasos, S.V.Lyulin, A.V.Lyulin  
*Journal of Materials Science B*, **2008**, 152, 114 (corresponding author)

**31. Investigation of Thermodynamic Properties of Hyperbranched Poly (ester amide) by Inverse Gas Chromatography**

G. S. Dritsas, K. Karatasos and C. Panayiotou  
*Journal of Polymer Science Part B: Polymer Physics* **2008**, 46, 2166

**32. "Dynamics of counterions in Dendrimer Polyelectrolyte Solutions"**

K. Karatasos and M. Krystallis  
*Journal of Chemical Physics* **2009**, 130, 114903

**33. "Molecular dynamics simulations of a hyperbranched poly(esteramide) : statics, dynamics and hydrogen bonding"**

I. Tanis, D. Tragoudaras, K.Karatasos and S. H. Anastasiadis  
*Journal of Physical Chemistry B*, **2009**, 113 (16), 5356

**34. "Electrostatically-driven Ordering in Model Dendrimer Polyelectrolytes: Effects of Concentration"**

K. Karatasos and M. Krystallis  
*Macromol. Symp.* , **2009**, 278, 32–39

35. **“Association of a weakly acidic anti-inflammatory drug (ibuprofen) with a poly(amidoamine) dendrimer as studied by molecular dynamics simulations”**  
I. Tanis and K. Karatasos  
*Journal of Physical Chemistry B*, **2009**, 113, 10984–10993.
36. **“Molecular dynamics simulations of polyamidoamine dendrimers and their complexes with linear poly(ethyleneoxide) at different pH conditions: static properties and hydrogen bonding”**  
I. Tanis and K. Karatasos  
*Physical Chemistry Chemical Physics*, **2009** 11, 10017–10028
37. **“Investigation of Thermodynamic Properties of Hyperbranched Aliphatic Polyesters by Inverse Gas Chromatography”**  
G. Dritsas, K. Karatasos and C. Panayiotou  
*Journal of Chromatography A*, 1216, (51), 8979-8985, **2009**
38. **Local Dynamics and Hydrogen Bonding in Hyperbranched Aliphatic Polyesters**  
I. Tanis and K. Karatasos  
*Macromolecules*, 42, 9581 , **2009**
39. **Modeling of Hyperbranched Polyesters as Hosts for the Multifunctional Bioactive Agent Shikonin**  
I. Tanis, K. Karatasos, A. N. Assimopoulou and V. P. Papageorgiou  
(corresponding author)  
*Physical Chemistry Chemical Physics*, 13, 10808, **2011**
40. **Aspects of PAMAM-based Dendrimer/siRNA complexation as studied by computer simulations: effects of pH and generation on dendrimer structure and siRNA binding**  
K. Karatasos, P. Posocco, E. Laurini, and S. Priel (corresponding author)  
*Macromolecular Bioscience*, **2012**, 12, p. 225
41. **Simulation of a symmetric binary mixture of charged dendrimers under varying electrostatic interactions: static and dynamic aspects**  
K. Karatasos and I. Tanis (corresponding author)  
*Macromolecules*, **2011**, 44, pp 6605
42. **Chimeric advanced drug delivery nano systems (chi-aSSnSs) for shikonin combining dendritic and liposomal technology**  
K. N. Kontogianopoulos, A. N. Assimopoulou, S. Hatziantoniou, K. Karatasos, C. Demetzos and V. P. Papageorgiou  
*International Journal of Pharmaceutics*, **2012**, 422, (1–2), 381-389
43. **Conformational effects in non-stoichiometric complexes of two hyperbranched molecules with a linear polyelectrolyte**  
G. Dalakoglou, K. Karatasos, S. Lyulin, S. Larin, A. Darinskii, A. Lyulin  
*Polymers* **2012**. 4,(1), 240-255 (corresponding author)
44. **Modeling the Formation of Ordered Nano-Assemblies Comprised by Dendrimers and Linear Polyelectrolytes: the Role of Coulombic Interactions**  
E. Eleftheriou and K. Karatasos  
*Journal of Chemical Physics*, **2012**, 137, 144905 (corresponding author)
45. **Tell Me Something I Do Not Know. Multiscale Molecular Modeling of Dendrimer/Dendron Organization and Self-Assembly In Gene Therapy.**

Posocco P, Laurini E, Col VD, Marson D, Karatasos K, Fermeiglia M, Pricl S.  
*Current Medicinal Chemistry*, 2012, 19, 5063-5067

- 46. Structure and Dynamics of Hyperbranched Polymer – Layered Silicate Nanocomposites**  
S. Fotiadou, C. Karageorgaki, K. Chrissopoulou, K. Karatasos, I. Tanis, D. Tragoudaras, B. Frick, and S. H. Anastasiadis  
*Macromolecules*, 2013, 46, 2842–2855
- 47. Self-association and Complexation of the Anti-Cancer Drug Doxorubicin with PEGylated Hyperbranched Polyesters in an Aqueous Environment**  
K. Karatasos  
*Journal of Physical Chemistry B*, 117, 2564-2575, 2013.
- 48. Complexes between poly(amido amine) dendrimers and poly(methacrylic acid): insight from molecular dynamics simulations**  
I. Tanis, K. Karatasos, P. Posocco, E. Laurini and S. Pricl (corresponding author)  
*MACROMOL SYMP* 2013, 331-332, (1), 34-42.
- 49. Graphene/Hyperbranched-Polymer Nanocomposites: Insight from Molecular Dynamics Simulations**  
K. Karatasos, *Macromolecules*, 47, (24), 8833-8845, 2014.
- 50. Detailed study of the dielectric function of a lysozyme solution studied with molecular dynamics simulations**  
Stelios Floros, Maria Liakopoulou-Kyriakides, Kostas Karatasos and Georgios E. Papadopoulos  
*European Biophysics Journal*, 44, (8), 599-611 2015
- 51. Graphene/ poly(ethylene glycol) nanocomposites as studied by molecular dynamics simulations**  
Roza-Eleftheria Roussou and Kostas Karatasos (corresponding author)  
*Materials & Design*, 97, 163-174, 2016
- 52. Characterization of a Graphene Oxide/Poly(acrylic acid) Nanocomposite by means of Molecular Dynamics Simulations**  
K. Karatasos and G. Kritikos (corresponding author)  
*RSC Advances*, 6, 109267, 2016
- 53. Frequency dependent non-thermal effects of oscillating electric fields in the microwave region on the properties of a solvated lysozyme system: a molecular dynamics study.**  
Stelios Floros; Maria Liakopoulou-Kyriakides; Kostas Karatasos; Georgios E Papadopoulos *PLoS ONE*, 2017, 12(1): e0169505
- 54. Temperature Dependence of Dynamic and Mechanical Properties in Poly(acrylic acid)/Graphene Oxide Nanocomposites**  
G. Kritikos and K. Karatasos  
*Materials Today Communications*, 2017, 13, 359-366
- 55. A microscopic view of graphene-oxide/poly(acrylic acid) physical hydrogels: effects of polymer charge and graphene oxide loading**  
K. Karatasos and G. Kritikos, *Soft Matter*, 2018, 14, 614-627 (corresponding author)
- 56. Nanostructure and Dynamics of Humidified Nafion-Graphene Oxide Composites via Molecular Dynamics Simulations**  
Kritikos, Georgios; Pant, Rakesh; Sengupta, Soumyadipta; Karatasos, Kostas; Venkatnathan, Arun; Lyulin, Alexey.  
*Journal of Physical Chemistry C*, 2018, 122, 22864-22875  
(corresponding author)

**57. Computational study of the interaction of a PEG-ylated hyperbranched polymer/doxorubicin complex with a bilipid membrane,** Prodomos Arsenidis, Kostas Karatasos, *Fluids*, **2019**, 4, 17 (corresponding author)

**58. Molecular dynamics simulation of the capillary leveling of a glass-forming Liquid**  
I. Tanis, K. Karatasos T. Salez, *The Journal of Physical Chemistry B*, **2019**, 123, 8543-8549

**59. Liposome-Templated Indocyanine Green J- Aggregates for In Vivo Near Infrared Imaging and Stable Photothermal Heating,** Calvin C. L. Cheung, Guanglong Ma, Kostas Karatasos, Jani Seitonen, Janne, Ruokolainen, Cédrik-Roland Koffi, Hatem A.F.M Hassan, and Wafa' T. Al-Jamal *Nanotheranostics*, **2020**, 4, 91-106 (front cover)

**60. Molecular Dynamics Simulations of Hydrated Poly(amidoamine) Dendrimer/Graphene-Oxide Nanocomposite Membranes,** K. Steiakakis and K. Karatasos *J. Phys. Chem. C* **2020**, 124, 9512-9522 (Corresponding author)

**61. Complexation of Single Stranded RNA with an Ionizable Lipid: an all-atom Molecular Dynamics Simulation Study,** Anastassia N. Rissanou Andreas Ouranidis, Kostas Karatasos *Soft Matter*, **2020**, 16, 6993-7005 (Corresponding author)

**62. Bound Layer Polymer Behavior on Graphene and Graphene Oxide Nanosheets**  
G. Kritikos, A. Rissanou, V. Harmandaris, and K. Karatasos, *Macromolecules*, **2020**, 53, 6190-6203

**h-index:** 24 (source: Scopus, Web of science), 26 (Google Scholar)

**Number of Citations:** 1750 (source: Scopus)

**Number of non-self citations:** over 1550 (source: Scopus)

#### **Chapters in books**

1. G.Fytas, K. Chrissopoulou, S. H. Anastasiadis, D. Vlassopoulos and K. Karatasos "Photon Correlation Spectroscopy of Interactive Polymer Systems" *NATO ASI, "Light Scattering and Photon Correlation Spectroscopy"* (E.R. Pike, ed.) Kluwer, N.Y (1997)
2. P. Posocco, E. Laurini, V. Dal Col, D. Marson, L. Peng, D.K. Smith, B. Klajnert, M. Bryszewska, A.-M. Caminade, J.P. Majoral, M. Fermeiglia, K. Karatasos and S. Prigl "Multiscale modeling of dendrimers and dendrons for drug and nucleic acid delivery" in *"Dendrimers in Biomedical Applications"*, *Royal Society of Chemistry*, ISBN: 978-1-84973-611-4 (2013), DOI:10.1039/9781849737296-00148, pp 148-166, 2013
3. Soumyadipta Sengupta, Alexey V. Lyulin, Giorgos Kritikos, Konstantinos Karatasos, Arun Venkatnathan, Rakesh Pant, Pavel Komarov *"Multiscale modelling examples: new polyelectrolyte nanocomposite membranes for perspective fuel and flow batteries"* Springer Series in Materials Science, vol 310, pp 133-177, Springer, Cham. [https://doi.org/10.1007/978-3-030-60443-1\\_6](https://doi.org/10.1007/978-3-030-60443-1_6), 2020

#### **Reviewer in International Journals:**

1. *Macromolecules*  
Recognized as among the top 25% of the reviewers of "Macromolecules" worldwide
2. *Journal of Chemical Physics*, (also adjudicator)
3. *Nanotechnology*
4. *Macromolecular Theory & Simulations*
5. *Journal of Polymer Science Part B: Polymer Physics*
6. *Physica B*
7. *Modelling and Simulation in Materials Science and Engineering*
8. *Journal of Physics: Condensed Matter*
9. *J. Phys. D: Appl. Phys*
10. *Rheologica Acta*
11. *New Journal of Physics*

12. European Polymer Journal E
13. Journal of Organic Chemistry
14. Chemistry - A European Journal
15. Journal of Physical Chemistry B
16. Measurement Science and Technology
17. Journal of Materials Chemistry
18. Journal of Physical Chemistry Letters
19. Journal of Polymer Research
20. European Physical Journal E - Soft Matter & Biological Physics
21. Molecules
22. Polymers
23. Journal of Drug Delivery Science and Technology
24. Soft Matter
25. ACS Applied Materials & Interfaces
26. Journal of Chemical Information and Modeling
27. ACS Nano
28. Journal of Molecular Graphics and Modeling
29. Chemical Science
30. Journal of Applied Polymer Science
31. International Journal of Molecular Sciences
32. Pharmaceuticals
33. Industrial & Engineering Chemistry Research
34. Molecular Therapy
35. Applied Physics Letters
36. International Journal of Nanomedicine
37. Bioconjugate Chemistry
38. Advances and Applications in Bioinformatics and Chemistry
39. Analytica Chimica Acta
40. Arabian Journal of Chemistry
41. Polymer Composites
42. Current Pharmaceutical Analysis
43. Biotechnology Advances
44. Environmental Science & Technology
45. Langmuir
46. Physical Chemistry Chemical Physics
47. The Arabian Journal for Science and Engineering
48. RSC Advances
49. Journal of Theoretical Biology
50. Nanomaterials
51. Nanoscale Research Letters
52. Current Pharmaceutical Design
53. Journal of Modern Physics
54. Current Clinical Pharmacology
55. Polymer Chemistry
56. Journal of the Neurological Sciences
57. Fluid Phase Equilibria
58. Journal of Computational Science
59. Composite Structures
60. Materials & Design
61. Computational Materials Science
62. Polymer
63. ACS Omega
64. Journal of Membrane Science
65. Chemical Physics Letters
66. Colloid and Polymer Science
67. ChemMedChem

**Guest Editor**

### **Reviewer in National and International Organizations**

European Science Foundations (ESF)  
Peer Reviewer of the Croatian Science Foundation (CSF)  
Peer Reviewer of the National Research Council of Romania (CNCS)  
Greek General Secretariat for Research and Technology (GSRT)  
Hellenic Foundation for Research & Innovation (H.F.R.I)  
Research Committee, University of Crete, Greece  
Hellenic Foundation for Research and Innovation (ELIDEK)

### **Invited Talks**

- 1. "Segmental dynamics and morphology in phase separated binary polymer blends"**  
*DIELECTRICA 98, Monte de Caparica, Portugal, June 1998*
- 2. "Short scale dynamics in Polyisobutylene"**  
Eindhoven University of Technology, The Netherlands, *June 2004*
- 3. "Statics and dynamics of model dendrimers in dilute solutions : a molecular dynamics study "**  
Free University of Brussels, Physics Department, Polymer Physics Group  
*Belgium, June 2004*
- 4. "Topological Aspects in Local Polymer Dynamics"**  
CECAM workshop on Simulating deformed glasses and melts: From simple liquids to polymers Organizers: A.V. Lyulin (Eindhoven), J.P. Wittmer (Strasbourg), D. Long (Paris) *CECAM, Lyon, France, 12-14 September 2005*
- 5. "Local Dynamics and Glass Transition in Polymers: the dendrimer case"**  
*HPC-Europa, Third Translational Access and Mobility Workshop (TAM ' 06) , Barcelona, Spain, June 14-16, 2006 (invited)*
- 6. "Controlling Self Organization in Dendrimer Polyelectrolytes"**  
*HPC-Europa, Fourth Translational Access and Mobility Workshop (TAM ' 07) , Bolonia, June 13-15, 2007 (invited)*
- 7. "Electrostatically-Driven Self-Organization in Dendrimer Polyelectrolytes"**  
*6th International Symposium Molecular Order and Mobility in Polymer Systems June 2 - 6, 2008, St. Petersburg Russia*
- 8. "Glass transition in "soft colloidal" systems: the dendrimer case"**  
Workshop on "Colloidal Gels and Glasses",  
Crete, Aldemar Knossos Royal Village, Hersonissos, 13/6/2008
- 9. "Molecular Dynamics of Dendrimers"**  
1<sup>st</sup> (ESF) International Training School in "Computer Simulation Methods of Dendrimers"  
12-14 April 2010, Eindhoven, The Netherlands (*plenary talk*)
- 10. Dendrimers and Hyperbranched Polymers: new insight from computer simulations**  
*Materials Science and Technology Department, University of Crete*  
25 February 2011 (*invited*)
- 11. Modeling Hyperbranched Polymers for Drug and Gene Delivery Applications**  
8<sup>th</sup> International Conference on Nanosciences & Nanotechnologies 12-15 July,

Thessaloniki, Greece (*invited*)

**12. Computer experiments in biomedical research: dendrimers and hyperbranched systems for drug and gene delivery purposes**

International training school and workshop on “*Dendrimers as Composites of Advanced Drug Delivery nano-Systems (aDDnSs). Biomedical Applications*” October 3-7, 2011, Athens, Greece (*invited*)

**13. Dendritic polymers as complexation agents for bioactive materials: a computational perspective**

Technical University of Eindhoven, Department of Applied Physics, March 25, 2013, Eindhoven, The Netherlands (*invited departmental seminar*)

**14. Hyperbranched polymers in nano-complexes: insight from computer simulations**

10th Hellenic Polymer Society Conference, 4-6 December 2014, Patras, Greece (*invited oral presentation*)

**15. Molecular Dynamics Simulations: a short introduction and applications in fully atomistic models of polymer-based systems for biomedical applications**

Workshop on «Mathematical and Computational Techniques for Molecular Systems»  
Institute of Applied and Computational Mathematics, FORTH, Heraklion, Crete, Greece  
16-18 September 2015  
(*invited keynote speaker*)

**16. Polymer-graphene nanocomposites: a close view by molecular dynamics simulations**

Institute of Macromolecular Compounds, St. Petersburg, 26/1/2016 (*invited seminar*)

**17. Graphene-based polymer nanohybrids from a computational perspective**

Department of Materials Science and Technology, University of Crete, Greece,  
6/3/2017 (*invited seminar*)

**18. Polyelectrolyte/Graphene-based nanocomposite hydrogels: a detailed view by molecular dynamics simulations**

12th Hellenic Polymer Society International Conference 2018, 30/9-3/10 2018, Ioannina, Greece (*invited talk*)

**19. Soft Matter Nanosystems in Biomedicine: An in-Silico Investigation**

(Invited Seminar) 20/1/2020

Foundation for Research and Technology – Hellas (FO.R.T.H), Institute of Electronic Structure and Laser

**Conference proceedings (refereed)**

1. S.H. Anastasiadis, K.Karatasos, G.Fytas, S.Pispas, M.Pitsikalis, N.Hadjichristidis, A.N Semenov, J.E.L Roovers, and T.Pakula  
“**Composition Fluctuation Effects on Dielectric Normal Mode Relaxation in Diblock Copolymer Melts**”  
*Polymer Prepr., Amer. Chem. Soc, Div. Polym. Chem. 35(1),608 (1994)*
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 Max Planck Institute for Polymer Research Mainz, Germany, 4-6 September 2000
33. K. Chrissopoulou, S. H. Anastasiadis, R. Krishnamoorti, K. Karatasos, G. Vlachos, E. Manias and E. P. Giannelis  
**"Polymer Dynamics under Nanoscopic Confinement"**  
*Euroconference on Chains @ Interfaces 2001, January 2001, Ivora, Portugal*
34. K. Karatasos and J.-P. Ryckaert  
**"Local dynamics of polyisobutylene revisited"**  
*Belgian Polymer Group, General Meeting 2001, 16-17 March, Sunparks Mol, Belgium*

35. K. Karatasos, and D.B. Adolf  
**“Effect of Density on Local Segmental Polymer Dynamics: A Molecular Dynamics Study “**  
*General Meeting , American Physical Society, March 2001,Seattle, USA*
36. S. Hotston, D. B. Adolf and K. Karatasos  
**“An NPT molecular dynamics study simulation of the response of the local segmental dynamics of melt polyethylene to pressure as a function of temperature “**  
*General Meeting , American Physical Society, March 2001,Seattle, USA*
37. K. Karatasos, D.B. Adolf and G. R. Davies  
**“Dynamics of model dendrimers as studied by molecular dynamics simulations “**  
*Polymer '01 The New Polymer: Design, Development and Applications 9-11 April 2001 Bath UK*
38. K. Karatasos and J-P. Ryckaert  
*4th International Discussion Meeting on Relaxations in Complex Systems*  
**"Methyl dynamics and  $\beta$ -relaxation in polyisobutylene as studied by molecular dynamics simulations"**  
*June 17-24 2001, Hersonissos, Crete, Greece*
39. K. Karatasos and J-P. Ryckaert  
*XVIII Hellenic Solid State and Material Science Conference, 15-18 September, 2002 Heraklion, Crete, Greece*  
**“Polyisobutylene local dynamics revisited”**
40. K. Chryssopoulou, K. Karatasos, S. H. Anastasiadis, E. Giannelis and B. Frick  
*XVIII Hellenic Solid State and Material Science Conference, 15-18 September, 2002 Heraklion, Crete, Greece*  
**“Dynamics of polymeric chains under strong confinement: motion in the nanometer scale”**
41. O. Ahumada, V. Arrighi, D.B.N. Coutrot, K. Karatasos, J.-P. Ryckaert, D. Theodorou, A. Triolo  
**QENS 2002.** The 6th International Conference on Quasielastic Neutron Scattering.  
 4th - 7th September 2002, Potsdam - Berlin, Germany.  
**"Effect of Tacticity on the Dynamics of Polypropylene Melts"**
42. K. Karatasos, J-P. Ryckaert  
 Jülich Soft Matter Days 19 - 22 November 2002, Kerkrade, NL
43. Kahle, S.; Monkenbusch, M.; Richter, D.; Ryckaert, J. P.\*; Karatasos, K.\*; Koza, M.\*  
**Segmental dynamics in polyisobutylene: comparison between neutron scattering and computer simulations**  
 Jülich Soft Matter Days 2002, Kerkrade, Niederlande, 19.11.2002 - 22.11.2002
44. Kahle, S.; Monkenbusch, M.; Richter, D.; Ryckaert, J. P.\*; Karatasos, K.\*; Koza, M.\*  
**Segmental dynamics in polyisobutylene: Comparison between neutron scattering and computer simulations**  
 HGF Workshop Kondensierte Materie : Forschungszentrum Jülich, Jülich, 06.11.2002
45. K. Chryssopoulou, K. Karatasos, S. H. Anastasiadis, E. P. Giannelis, B. Frick  
**"Dynamics under severe confinement in intercalated polymer-clay nanocomposites: Motion in the nanometer scale"**  
 2nd International Workshop on ' DYNAMICS IN CONFINEMENT', January 2003, Grenoble, France
46. K. Karatasos, D. B. Adolf and G. Davies

**"Static and dynamic properties of model dendrimers"**

3<sup>rd</sup> Chemical Engineering Conference for Collaborative Research in Eastern Mediterranean, 13-15 May 2003, Sani, Chalkidiki

47. K. Chrissopoulou, K. Karatasos, S. H. Anastasiadis, E. P. Giannelis, B. Frick  
« **Effects of strong spatial confinement in polymer chain dynamics** »  
4<sup>th</sup> Hellenic conference in Chemical Engineering, Patras, May 2003
48. Marras, S, Zoubourtikoudis, I, Karatasos, K, Sikalidis, K and Panayiotou, K.  
"Development of novel nanocomposite biodegradable polymer materials"  
XX Panhellenic Conference in Solid State Physics and Materials Science  
Ioannina, September 2004, Greece
49. K. Chrissopoulou, K. Karatasos, S.H. Anastasiadis, E.P. Giannelis and B. Frick,  
" **Dynamics in Intercalated Polymer-Clay Nanocomposites** "  
11th European Conference on Composite Materials May 31 - June 3, Phodes, Greece  
(Conference Proceedings, Vol 1/2 , p. 81)
50. JP Ryckaert, G. Ariedi, K. Karatasos  
" **Local Dynamics in Polymer Melts : From Individual Jumps to Diffusive Coarse-Grained Dynamics** "  
Conference on Computational Physics 2004 Genoa Italy, 1-4 September 2004  
(Invited)
51. Ryckaert, J.-P., Ariedi G. , Karatasos K.  
" **From local dynamics to conformational diffusion in polymer melts well above T<sub>g</sub>** "  
N2M2 Neutron and Numerical Methods 2, Institute Laue Langevin, September 2004,  
Grenoble, France (invited)
52. K. Karatasos  
" **Statics and dynamics in model dendrimer melts: toward the glass transition** "  
5<sup>th</sup> Panhellenic Scientific Conference in Chemical Engineering  
Thessaloniki, May 26-28 2005, Greece
- 53 . K. Karatasos  
" **Topological Aspects in Local Polymer Dynamics** "  
CECAM workshop on Simulating deformed glasses and melts: From simple liquids to  
polymers Organizers: A.V. Lyulin (Eindhoven), J.P. Wittmer (Strasbourg), D. Long  
( Paris) *CECAM, Lyon, France, 12-14 September 2005 (invited)*
54. K. Karatasos  
" **Statics and Dynamics in Model Dendrimer Melts** "  
2006 APS March Meeting, March 13-17, Baltimore, Maryland, U.S.A.
55. AERC 2006, Third Annual European Rheology Conference, April 27-29, Hersonissos,  
Crete, 2006
56. K. Karatasos  
" **Local Dynamics and Glass Transition in Polymers: the dendrimer case** "  
HPC-Europa, Third Translational Access and Mobility Workshop (TAM ' 06) ,  
Barcelona, Spain, June 14-16, 2006
57. K. Karatasos  
" **Glassy Behavior in Nanoscale Dendritic Polymers** "  
*3<sup>rd</sup> Workshop on Nanoscience & Nanotechnologies (N&N06), 10-12 July, 2006,  
Thessaloniki, Greece*
58. K. Karatasos  
" **Local Scale Dynamics in Model Dendrimer Melts** "  
6<sup>th</sup> Hellenic Conference on Polymers, Patras, 3-5 November 2006

59. G.K. Dalakoglou, K. Karatasos, S. Lyulin, A. Lyulin  
**“Brownian Dynamics Simulations of Complexes of HYperbranched Polymers with Linear Polyelectrolytes”**  
6<sup>th</sup> Panhellenic Chemical Engineering Scientific Conference, Athens, May 2007
60. K. Karatasos  
**“Controlling Self Organization in Dendrimer Polyelectrolytes”**  
HPC-Europa, Fourth Translational Access and Mobility Workshop (TAM ‘ 07) ,  
Bologna, Italy, June 13-15, 2007 (*invited*)
- 60b. I. Tanis, K. Karatasos  
**“Atomistic molecular dynamics simulations of dendrimers and their complexes with linear polyelectrolytes”**  
HPC-Europa, Fourth Translational Access and Mobility Workshop (TAM ‘ 07) ,  
Bologna, Italy, June 13-15, 2007
61. G.K. Dalakoglou, K.Karatasos, S.V.Lyulin, A.V.Lyulin  
**“Brownian Dynamics Study of Hyperbranched Polymers and their Complexes with Linear Polyelectrolytes: Effects of Topology and Electrostatic Interactions”**  
4th International Workshop on “Nanosciences & Nanotechnologies - NN07,  
July 16-18, Thessaloniki, Greece, 2007
- 61b. G.S. Dritsas, I. Tanis, K. Karatasos, C. Panayiotou  
**“Investigation of Thermodynamic Properties of a Poly(amidoamine) Dendrimer by Inverse Gas Chromatography and Computer Simulations”**  
4th International Workshop on “Nanosciences & Nanotechnologies - NN07,  
July 16-18, Thessaloniki, Greece, 2007
62. K. Karatasos  
**“Controlling self-organization in Dendrimer Polyelectrolytes”**  
Soft, Complex, and Biological Matter Conference Citta del Mare, Terrasini, Sicily  
July 2007
63. I. Tanis and K. Karatasos  
**“Atomistic molecular dynamics simulations of dendrimers and their complexes with linear polyelectrolytes”**  
XXIII Panhellenic Conference in Solid State and Materials Science,  
23-26 September 2007, Athens, Greece
64. K. Karatasos, G. Dalakoglou, I. Tanis and M. Krystallis  
**“Computer Simulations in Complex Polymeric Systems”**  
1<sup>st</sup> HellasGrid User Forum Meeting, Athens 10-11 Jan. 2008
65. S. Lyulin, A. Lyulin, S. Larin, A. Darinskii, K. Karatasos  
**“Charged dendrimers and their complexes with linear polyelectrolytes: insight from coarse-grained molecular dynamics simulations”**  
Hyper-Nano 2008, May 26-28, Fodele, Crete, Greece
- 65b. G.K. Dalakoglou, K. Karatasos, S.V. Lyulin, A.V. Lyulin  
**“Shear-induced effects in complexes formed by hyperbranched polymers and linear polyelectrolytes”**  
Hyper-Nano 2008, May 26-28, Fodele, Crete, Greece
- 65c. G.S. Dritsas, K. Karatasos, C. Panayiotou  
**“Investigation of thermodynamic properties of hyperbranched poly(ester amide) by inverse gas chromatography”**  
Hyper-Nano 2008, May 26-28, Fodele, Crete, Greece
- 65d. D. Tragoudaras, I. Tanis, K. Karatasos, S. Anastasiadis

- “Molecular dynamics simulations of a hyperbranched poly(ester amide), Hybrane “**  
Hyper-Nano 2008, May 26-28, Fodele, Crete
66. K. Karatasos  
**“Electrostatically-driven self-organization in dendrimer polyelectrolytes”**  
6th International Symposium in Molecular Order and Mobility in Polymer Systems  
St. Petersburg, 2-6 June 2008, Russia.
- 66b. S.V. Lyulin, K. Karatasos, S.V. Larin, A.A. Darinskii, A.V. Lyulin  
**“Charge inversion in complexes of hyperbranched polymers and oppositely charged linear polyelectrolytes”**  
6th International Symposium in Molecular Order and Mobility in Polymer Systems  
St. Petersburg, 2-6 June 2008, Russia.
67. K. Karatasos  
**“Glass transition in "soft colloidal" systems: the dendrimer case”**  
Workshop on “Colloidal Gels and Glasses”,  
Crete, Aldemar Knossos Royal Village, Hersonissos, 13/6/2008
68. G. K. Dalakoglou, K. Karatasos, S.V. Lyulin, A.V. Lyulin  
**Modelling of Complexes of Hyperbranched Polymers with Linear Polyelectrolytes in Shear Flows**  
5<sup>th</sup> International Conference on Nanosciences and Nanotechnologies (N&N08)  
Thessaloniki 14-16 July 2008 ,
69. K. Karatasos and M. Krystallis  
**Self-Ordering in Model Dendrimer Polyelectrolytes**  
1<sup>st</sup> International Conference “From Nanoparticles & Nanomaterials to Nanodevices & Nanosystems”  
Halkidiki, Greece, June 16-18, 2008
70. I. Tanis, K. Karatasos  
**Molecular dynamics of PAMAM dendrimers and their complexes with linear polymers in aqueous solutions**  
7th Hellenic Polymer Conference, Ioannina, September 28th - October 1st 2008
- 70b. G. S. Dritsas, I. Tanis, M. Stournara, K. Karatasos, C. Panayiotou  
**Investigation of thermodynamic properties of polyethylene glycol by inverse Gas chromatography and computer simulations**  
7th Hellenic Polymer Conference, Ioannina, September 28th - October 1st 2008
71. S. Fotiadou, D. Tragoudaras, I. Tanis, K. Chrissopoulou, K. Karatasos, B. Frick and S.H. Anastasiadis  
**Structure and dynamics of hyperbranched polymers: A comparison between experiment and simulation**  
XXIV Panhellenic Conference on Solid State Physics and Materials Science  
Heraklion, Crete, September 21-24, 2008, Book of Abstracts, P. 62-63
72. Karatasos and M. Krystallis  
**STATICS AND DYNAMICS IN COULOMBIC-DRIVEN ORDERING IN MODEL DENDRIMER POLYELECTROLYTES: A MOLECULAR DYNAMICS SIMULATION STUDY**  
7<sup>th</sup> Panhellenic Chemical Engineering Scientific Conference, Patras, 3-5 June 2009
73. K. Karatasos and I. Tanis  
**Complexes of Poly(amidoamine) dendrimers in aqueous solutions as studied by molecular dynamics simulations**  
6<sup>th</sup> International Dendrimer Symposium 2009, Stockholm, Sweden, 14-18 June 2009

74. KOSTAS KARATASOS, SABRINA PRICL , PAOLA POSOCCO,ERIK LAURINI  
**A MOLECULAR DYNAMICS SIMULATION STUDY ON SI-RNA/TEA-PAMAM DENDRIMER COMPLEXATION**  
**8<sup>TH</sup> HELLENIC POLYMER SOCIETY SYMPOSIUM , HERSONISSOS CRETE, 24 – 29 OCTOBER, 2010**
75. Pricl, P. Posocco, M. Fermeglia, K. Karatasos, L. Peng and D. K. Smith  
**The Sound of Silence. Multiscale Molecular Simulations and Experiments in Developing Nanocarrier/Nucleic Acid Systems**  
 AIChE Annual Meeting, 2010, Salt Lake City, November 7-10, 2010
76. S. Pricl, P. Posocco, E. Laurini, M. Fermeglia, K. Karatasos, L. Peng and D. K. Smith  
**When virtual and real meet: computational/experimental evidences for designing efficient nanovectors for siRNA/DNA delivery**  
 NanoTechItaly 2010, Venice, October 20-22, 2010
77. K. Karatasos, P. Posocco, E. Laurini and S. Pricl  
**Computational study of complexes of Dendrimers with siRNA for gene delivery applications**  
 8th Panhellenic Scientific Chemical Engineering Congress, Thessaloniki 26 - 28 May 2011, Greece
78. K. Karatasos  
**Modeling Hyperbranched Polymers for Drug and Gene Delivery Applications**  
 8<sup>th</sup> International Conference on Nanosciences & Nanotechnologies 12-15 July, Thessaloniki, Greece, 2011
79. K. Karatasos and E. Eleftheriou  
**Modeling the formation of nanogels comprised by dendrimer polyelectrolytes under the influence of varying electrostatic interactions**  
 9<sup>th</sup> International Conference on Nanosciences & Nanotechnologies 3-6 July, Thessaloniki, Greece, 2012
80. K. Karatasos and E. Eleftheriou  
**Modeling the Formation of Ordered Nano-Assemblies Comprised by Dendrimers and Linear Polyelectrolytes: the Role of Coulombic Interactions**  
 9th Hellenic Polymer Society Conference (Polymers 2012) 29 November - 1 December 2012, Thessaloniki, Greece
81. K. Karatasos  
**Self-Association and Complexation of the Anti-Cancer Drug Doxorubicin with PEGylated Hyperbranched Polyesters in an Aqueous Environment**  
 10<sup>th</sup> International Conference on Nanosciences & Nanotechnologies 9-12 July 2013, Thessaloniki, Greece
82. Anastasiadis, S. H.; Chrissopoulou, K.; Karatasos, K.; Fotiadou, S.; Karageorgaki, C.; Tanis, I.; Tragoudaras, D.; Frick, B.  
**Structure and dynamics of hyperbranched polymers in bulk and under nanoscopic confinement**  
*American Physical Society*, March 2013, Baltimore, MD, U.S.A.
83. Chrissopoulou, K.; Fotiadou, S.; Tanis, I.; Karatasos, K.; Frick, B.; Anastasiadis, S. H.  
**Dynamics of Dendritic Polymers in the Bulk and under Confinement**  
*European Polymer Congress 2013*, June 2013, Pisa, Italy
84. Chrissopoulou, K.; Fotiadou, S.; Androulaki, K.; Tanis, I.; Karatasos, K.; Prevosto, D.; Labardi, D.; Frick, B.; Anastasiadis, S. H.  
**Dynamics of Hyperbranched Polymers in the Bulk and Under Confinement**  
 QENS/WINS2014, May 2014, Autrans, France

85. Chrissopoulou, K.; Fotiadou, S.; Androulaki, K.; Tanis, I.; Karatasos, K.; Prevosto, D.; Labardi, M.; Frick, B.; Anastasiadis, S. H.  
**Dynamics of Dendritic Polymers Polymers in the Bulk and under Confinement**  
 Times of Polymer and Composites TOP 2014, June 2014, Ischia Italy
86. K. Karatasos  
**Molecular Dynamics Simulations of Graphene/Hyperbranched-Polymer Nanocomposites**  
 11th International Conference on Nanosciences & Nanotechnologies (NN14)  
 8-11 July 2014, Thessaloniki, Greece
87. K. Karatasos  
**Graphene/Polymer Nanocomposites: insight from Molecular Dynamics Simulations**  
 Workshop “Applications of Hybrid Materials Interfaces” of COST action MP1202,  
 “RATIONAL DESIGN OF HYBRID ORGANIC-INORGANIC INTERFACES: THE NEXT STEP TOWARDS ADVANCED FUNCTIONAL MATERIALS”  
 15-17 September 2014, Istanbul, Turkey
88. K. Karatasos  
**“Hyperbranched Polymers in Nano-Complexes: Insight from Computer Simulations”**  
*10th Hellenic Polymer Society Conference, Patras, 4-6 December 2014, Greece*
89. K. Karatasos and R.-E. Roussou  
**Characterization of the dispersion of graphene nanosheets in poly(ethylene glycol) by molecular dynamics simulations**  
 Workshop on “Nanostructured Hybrid Materials II: reinforced 3D structures, smart composites, Self-healing” of COST action MP1202,  
 “RATIONAL DESIGN OF HYBRID ORGANIC-INORGANIC INTERFACES: THE NEXT STEP TOWARDS ADVANCED FUNCTIONAL MATERIALS”  
 22-24 April 2015, Heraklion, Crete, Greece
90. K. Karatasos and R.-E. Roussou  
**Effects of Macromolecular Architecture and Size on Polymer/Graphene Nanocomposites: Insight from Molecular Dynamics Simulations**  
 XXXI Panhellenic Conference on Solid State Physics and Materials Science  
 20-23 September 2015, Thessaloniki, Greece
91. S. Floros, M. Liakopoulou-Kyriakides, K. Karatasos and G. E. Papadopoulos  
**Dielectric study of a lysozyme solution with molecular dynamics simulations: Non thermal effects of low alternating electric fields**  
 XXXI Panhellenic Conference on Solid State Physics and Materials Science  
 20-23 September 2015, Thessaloniki, Greece
92. K. Karatasos  
**Molecular Dynamics Simulations: A short introduction and applications in fully atomistic models of polymer-based systems for biomedical applications**  
 Workshop on «Mathematical and Computational Techniques for Molecular Systems» Institute of Applied and Computational Mathematics, FORTH,  
 Heraklion, Crete, Greece 16-18 September 2015
93. . Ioannis Tanis, Thomas Salez, Anthony Maggs, Kostas Karatasos  
**Static and dynamic aspects of a stepped liquid film as studied by MD simulations**  
 STATPHYS26 - PALAIS DES CONGRES - LYON 18-22 JULY 2016
94. Stelios Floros, Maria Liakopoulou-Kyriakides, Kostas Karatasos and Georgios E. Papadopoulos

**Microwave non-thermal effects of a solvated lysozyme system: a molecular dynamics study**

Joint International Conference of the Hellenic Crystallographic Association and the Hellenic Society for Computational Biology and Bioinformatics  
HeCrA-HSCBB16, October 7-9, 2016, Athens, Greece

95. K. Karatasos and G. Kritikos

**Graphene oxide – Poly(acrylic acid) nanocomposites as studied by molecular dynamics simulations**

*11th Hellenic Polymer Society Conference*, Heraklion, 3-5 November 2016, Greece

96. I. Tanis, T. Salez, K. Karatasos, A.C. Maggs,

**Static and dynamic aspects of a liquid film bearing a nonconstant surface topography as studied by molecular dynamics simulation**

*Liquids@Interfaces*, 17-19 October 2016, Paris, France

97. K. Karatasos and G. Kritikos

**Structure and Dynamics in Polymer/Graphene-based Nanocomposites as Studied by Molecular Dynamics Simulations**

*Eurofillers Polymer Blends*, 24-27 April 2017, Chersonissos, Crete, Greece

98. I. Tanis, T. Salez, K. Karatasos, A.C. Maggs

**RELAXATION OF LIQUID FILMS BEARING A NON-CONSTANT SURFACE TOPOGRAPHY AS STUDIED BY MOLECULAR DYNAMICS SIMULATIONS**

*11th Panhellenic Conference on Chemical Engineering*  
May 25-27, Thessaloniki, Greece, 2017

99. G. Kritikos and K. Karatasos

**Study of poly(acrylic acid)/Graphene Oxide nanocomposites by means of molecular dynamics simulations**

*11th Panhellenic Conference on Chemical Engineering*  
May 25-27, Thessaloniki, Greece, 2017

100. M. Belioka, K. Androulaki, I. Tsivintzelis, K. Chrissopoulou and K. Karatasos

**Preparation and characterization of poly(vinyl alcohol)/montmorillonite nanocomposite hydrogels**

*11th Panhellenic Conference on Chemical Engineering*  
May 25-27, Thessaloniki, Greece

101. M. Belioka, K. Androulaki, I. Tsivintzelis, K. Chrissopoulou and K. Karatasos

**Preparation and Characterization of Poly(Vinyl alcohol)/Na+Montmorillonite Nanocomposite Hydrogels**

*14th International Conference on Nanosciences & Nanotechnologies (NN17)*  
4-7 July 2017, Thessaloniki, Greece,

102. Stelios Floros, Maria Liakopoulou-Kyriakides, Kostas Karatasos and Georgios E. Papadopoulos

**Dielectric properties and non thermal effects of microwaves on lysozyme studied with molecular dynamics simulations**

*14th International Conference on Nanosciences & Nanotechnologies (NN17)*

103. Soumyadipta Sengupta, Giorgos Kritikos, Konstantinos Karatasos, Arun Venkatnathan, Rakesh Pant, Pavel Komarov and Alexey V. Lyulin

**Novel Polyelectrolyte Membranes for Fuel and Flow Batteries: Insights from Simulations**

*9th Conference on "Times of Polymers (TOP) & Composites"*  
June 18-21 2018, Ischia, Italy

104. K. Karatasos and G. Kritikos

Polyelectrolyte/graphene—based nanocomposite hydrogels: a detailed view by molecular dynamics simulations  
12 Hellenic Polymer Society Conference  
September 30-October 3 2018, Ioannina, Greece

105. M. Belioka, K. Androulaki, I. Tsivintzelis, K. Chrissopoulou and K. Karatasos  
**Preparation and characterization of poly(vinyl alcohol)/montmorillonite nanocomposite hydrogels**  
11th Panhellenic Conference on Chemical Engineering  
May 25-27, Thessaloniki, Greece, 2017
106. M. Belioka, K. Androulaki, I. Tsivintzelis, K. Chrissopoulou and K. Karatasos  
**Preparation and Characterization of Poly(Vinyl alcohol)/Na+Montmorillonite Nanocomposite Hydrogels**  
14th International Conference on Nanosciences & Nanotechnologies (NN17)  
4-7 July 2017, Thessaloniki, Greece,
107. Stelios Floros, Maria Liakopoulou-Kyriakides, Kostas Karatasos and Georgios E. Papadopoulos  
**Dielectric properties and non thermal effects of microwaves on lysozyme studied with molecular dynamics simulations**  
14th International Conference on Nanosciences & Nanotechnologies (NN17),  
4-7 July 2017, Thessaloniki, Greece
108. Soumyadipta Sengupta, Giorgos Kritikos, Konstantinos Karatasos, Arun Venkatnathan, Rakesh Pant, Pavel Komarov and Alexey V. Lyulin  
**Novel Polyelectrolyte Membranes for Fuel and Flow Batteries: Insights from Simulations**  
9th Conference on "Times of Polymers (TOP) & Composites"  
June 18-21 2018, Ischia, Italy
109. K. Karatasos and G. Kritikos  
**Polyelectrolyte/graphene—based nanocomposite hydrogels: a detailed view by molecular dynamics simulations**  
12 Hellenic Polymer Society Conference  
September 30-October 3 2018, Ioannina, Greece
110. K. Steiakakis and K. Karatasos  
**Molecular Dynamics Simulations of Humidified Nanocomposites of Graphene Oxide with Poly(amidoamine) dendrimers**  
12th Panhellenic Conference on Chemical Engineering  
May 29-31, Athens, Greece, 2019
111. Bacova, Eirini Gkolfi, Emmanouil Glynos, Kostas Karatasos, Vagelis Harmandaris and Spiros H. Anastasiadis  
**“Molecular insight into the internal morphology and dynamics of polystyrene stars”** Annual European Rheology Conference 2019 (AERC 2019),  
Portoroz/Slovenia, April 8 – 11, 2019
112. Georgios Kritikos, Rakesh Pant, Soumyadipta Sengupta, Kostas Karatasos, Arun Venkatnathan and Alexey Lyulin  
**“Humidified Nafion/Graphene-Oxide Composites as Studied by Molecular Dynamics Simulations”**  
European Polymer Congress, June 9-14, 2019, Hersonissos, Crete, Greece
- 112b. Eirini Gkolfi, Petra Bacova, Kostas Karatasos, Vagelis Harmandaris  
**“Atomistic study of star-shaped polystyrene melts”**  
European Polymer Congress, June 9-14, 2019, Hersonissos, Crete, Greece
113. N. Rissanou, V. Harmandaris, K. Karatasos and A. Ouranidis

## **“Structure and Self-Assembly of Biomolecules through Molecular Simulations”**

16th International Conference on Nanosciences & Nanotechnologies (NN19)  
2-5 July 2019, Thessaloniki, Greece

114. I.Tanis, K. Karatasos, T. Salez

### **“Molecular dynamics simulation of the capillary leveling of a glass-forming liquid”,**

Journées de Physique Statistique 2020, 30-31 January, ENS Paris, France

## **Participation in International Collaborative Research Projects**

1. Brite-Euram: “Reactive Blends : a new way for improved and recycled materials”
2. NATO’s Scientific Affairs: Science for Stability Programme
3. Brite-Euram: “Polymer Blends with optimized properties : influence of Processing and additives on phase behavior”
4. “Theoretical and Experimental Investigations of the Structure and Mobility of Polymer Networks”, INTAS Contract: 932502
5. TMR network “New routes to understanding polymer materials using experiments and realistic modeling”
5. Marie-Curie Host Fellowship for the Transfer of Knowledge (ToK) “*Colloidal Systems in Non-Ergodic States*” (COSINES), 2006-2010
6. Project COST, European Science Foundation (TD0802) “*Biomedical applications of Dendrimers*” (2009-2013) ( Greek representative in the Management Committee)
7. Project COST, European Science Foundation (MP1202) “*Rational Design of Hybrid Organic-Inorganic Interfaces: the next step towards Advanced Functional Materials*” 2013-2016
8. Project COST της European Science Foundation (CA17140) “*Nano2Clinic : Cancer Nanomedicine – from the bench to the bedside*” 2018-2021

## **Participation in other projects**

1. Microporous composites of biopolymers with hydroxyapatite for bone replacement and controlled drug release (*Greek Ministry of Education and Religious Affairs, “Pythagoras”, 2004*)
2. Examination of nanosystems of hyperbranched polymers and their complexes as solubility enhancement agents and vehicles for controlled releases of drug molecules and biomaterials *PENED* 2003, GSRT, 2005-2008 (Principal Investigator, Budget 198000€)
3. HPC-EUROPA project (RII3-CT-2003-506079) “**Topological Aspects of Polymer Glass Transition**”), with the support of the European Community - Research Infrastructure Action under the FP6 "Structuring the European Research Area" Programme (15000 CPU Hours - COMPUTER TIME GRANT, SARA Supercomputing Center, Amsterdam, The Netherlands) 2005
4. HPC-EUROPA project (RII3-CT-2003-506079) “*Controlling self-organization in Dendrimer Polyelectrolytes*”), with the support of the European Community - Research Infrastructure Action under the FP6 "Structuring the European Research Area" Programme (20000 CPU Hours, Edinburgh Supercomputing Center, Edinburgh, England - COMPUTER TIME GRANT) 2007
5. HPC-Europa 2 project, funded by the European Commission - DG Research in the 7<sup>th</sup> Framework Programme ( Grant agreement n° 228398) (100000 CPU Hours, COMPUTER TIME GRANT , CINECA Supercomputing Center, Bolonia, Italy) “*A fully atomistic molecular dynamics study of dendrimer/gene complexation in aqueous environment*” 2010
6. HPC-Europa 2 project, funded by the European Commission - DG Research in the 7<sup>th</sup> Framework Programme ( Grant agreement n° 228398) (150000 CPU Hours, COMPUTER TIME GRANT , CINECA Supercomputing Center, Bolonia, Italy) « *Study of a novel polymer-based nanocarrier for the anticancer drug doxorubicin* » 2012

7. “*High performance nanocomposite materials: Reinforcement of polymers with advanced carbon and silica nanostructures*” “THALIS” ESPA 2010-2013 (participation in the research team, AUTH)
8. “*NANO4HEALTH*” Standard HPC Grant 2012, CINECA Supercomputing Center, Bologna, Italy (March 2012 – March 2013) (coordinator: Prof. S. Pricl, University of Trieste, Dept. of Engineering and Architecture).
9. “*HERON-A : Hierarchical in-silico EngineeRing of Optimized vectors for Nanomedical Applications*” (coordinator, IS CRA C project, CINECA Supercomputing Center, Bologna, Italy, March 2013-March 2014)
10. “*Nanogels in regenerative medicine – non-invasive application in tissue engineering*” 1/1/2014-31/12/2014, (member of the research team) , Latsis Foundation, Budget:12000€
11. “*GOPOLY*”, Molecular dynamics simulations of conductive hydrogels based on graphite oxide and poly(acrylic acid) (coordinator, 1500000 CPU hours computing time, ARIS Hellenic Supercomputing Center, Athens, 1/6/2016-1/6/2017)
12. “*NANOGRAPH*” Statics, dynamics and interfacial phenomena in polymer/Graphene-based nanocomposites (member of a collaborative team, 4000000 CPU hours computing time, ARIS Hellenic Supercomputing Center, Athens,17/2/2017-now)
13. “*DENDRIGO*” Graphene oxide/dendrimer polyelectrolyte membranes:effects of dendrimer generation in their physical properties (coordinator, 1750000 CPU hours computing time, ARIS Hellenic Supercomputing Center, Athens, 2018)
14. «*NY2Π*» Novel Nano Superparamagnetic Navigators (NY2Π<sub>ς</sub>) of Ribonucleic proteins for personalized breast cancer treatment « Entrepreneurship and Innovation, under the call RESEARCH – CREATE – INNOVATE 2014-2020», Code T1EΔK-02775, 2018-2021, member of the research team, PI of a subproject with budget 98000€
15. «*Aroma distil*» Exploitation of aromatic and pharmaceutical plants of Greek flora , Entrepreneurship and Innovation, under the call RESEARCH – CREATE – INNOVATE, Code T1EΔK-04174, 2018-2021, member of the research team
16. «*NAPPY*» Nano-reinforced polypropylene yarns, Operational Programme Competitiveness, Entrepreneurship and Innovation (EPAnEK 2014-2020), 2019-2022, member of the research team.
17. «*POLYGRAPH*» Polymer / graphene derivative materials: Effect of interfacial interactions on the structure and properties of the polymer 2019-2021 (Deputy Academic Advisor) Operational Program "Human Resources Development, Education and Lifelong Learning" (EΠ ANAA-EΔBM), ESPA 2014-2020

### **Other Grants/Fellowships**

1. Greek National Scholarship Foundation Fellowship 1988,1989,1990,1991.
2. European Community, Erasmus 1991
3. FO.R.T.H-IESL, Graduate Research Fellowship 1992-1997
4. *HPC-Europa*, Personal,Computer Time Grant (20000 CPU hours) *Septemper 2005*

5. *HPC-Europa*, , Personal, Computer Time Grant (20000 CPU hours) *January 2007*
6. European Science Foundation (ESF) grant for the organization of the ESF international exploratory workshop "HYPER-NANO 2008" Grant: 14000 € (**Principal Organizer**)
7. Greek Ministry for National Education and Religious Affairs, grant for the organization of "HYPER-NANO 2008" Grant: 5000 € (**Principal Organizer**)

### **Conference/Meeting Organization**

1. *International Workshop*, under the auspices of the European Polymer Federation and the European Science Foundation (Funding Body)  
 “*Hyperbranched polymers as novel materials for nanoscale applications : insight from experiment, theory and simulations (HYPER-NANO)*” May 26-28, 2008,  
 Fodele, Grete, Greece  
 Web-site: <http://users.auth.gr/~kkaratas/workshop>  
Organizers: K.Karatasos (principal), A.V.Lyulin
2. 1<sup>st</sup> International Training School, “*Computer Simulation Methods for Dendrimers*”, 12-10 April 2010, Eindhoven, The Netherlands (funded by ESF)  
Organizers: A.V.Lyulin (principal), K.Karatasos (Co-organizer)  
 Web-site: <http://physlamp.phys.tue.nl/COST/>
3. Member of the Organization Committee of the International School in *Dendrimers as Composites of Advanced Drug Delivery nano Systems αDDnSs*. *Biomedical Applications* October 4-9, Athens, 2011, Greece (under the auspices of and funding from the European Science Foundation)
4. Member of the Organizing Committee of the 8<sup>th</sup> meeting of the Hellenic Polymer Society November 2012, Thessaloniki, Greece
5. Member of the Scientific Committee, 9<sup>th</sup> Hellenic Chemical Engineering Conference, Athens 23-25 May, 2013
6. Member of the Organizing and the Scientific Committee, 10<sup>th</sup> Hellenic Polymer Society Conference, Patras, December 2014
7. Member of the Scientific Committee, 11<sup>th</sup> Hellenic Polymer Society Conference, Heraklion, November 2-5, 2016
8. Member of the Scientific Committee, 11<sup>th</sup> Hellenic Chemical Engineering Conference, Thessaloniki 25-27 May, 2017
9. Member of the Scientific Committee, 12<sup>th</sup> International conference of the Greek Polymer Society, Ioannina, Greece, September 30-October 3 2018
10. Member of the organizing and the scientific committee of the «*Eurofillers Polymer Blends*» international conference, 2017, April 23-27, Crete, Greece
11. Member of the Scientific Committee, 12<sup>th</sup> Hellenic Chemical Engineering Conference, Ioannina 30/9-3/11 2018
12. Member of the organizing committee of the European Polymer Congress (EPF), 2019, Crete, Greece
13. Member of the organizing committee of the European Colloid and Interfaces Conference (ECIS), 2021, Crete, Greece

### **Visits (with stay) to international research institutes**

- 4/1991-7/1991 University of Amsterdam, Astronomical Institute «Anton Pannekoek» .
- 2/1994-3/1994 Max-Planck Institute für Polymerforschung
- 5/1995 National Institute of Standards and Technology (USA)
- 6/1995 University of Leipzig
- 9/2000 Institute Laue-Langevin, Grenoble, France
- 12/2000 Herriot-Watt University, Edinburgh, Scotland
- 11/2003 Université Libre Des Bruxelles
- 6/2004 Technical University of Eindhoven
- 9/2005 Technical University of Eindhoven
- 1/2007 Center for Self Organization of Molecular Species (SOMS), Leeds, UK
- 2/2010-6/2010 University of Trieste, Italy
- 1/2013 University of Trieste, Italy
- 1/2016 Institute of macromolecular compounds, St. Petersburg, Russia

### **Other Qualifications**

***Experimental Techniques*** : Dielectric Spectroscopy, Dynamic Light Scattering, Differential Scanning Calorimetry (DSC), Neutron Scattering

***Computer Operating systems***: Unix (including experience in HPC Facilities), Linux, Ms-Windows

***Experience in usage of simulation packages***: DL\_POLY, DL\_PROTEIN, Accelrys Materials Studio, NAMD

***Programming Languages*** : C, FORTRAN, Pascal