

ΒΙΟΓΡΑΦΙΚΟ ΣΗΜΕΙΩΜΑ

Κωνσταντίνου Δ. Καρατάσου
Επ. Καθηγητή του Τμ. Χημικών Μηχανικών, Α.Π.Θ.

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ΘΕΣΣΑΛΟΝΙΚΗ ΙΑΝΟΥΑΡΙΟΣ 2012

Διαθέσιμη επικαιροποιημένη έκδοση από τον σύνδεσμο
<http://users.auth.gr/kkaratas/cvkaratasosgr.pdf>

Επαγγελματική πορεία

- 1969 : Έτος γέννησης
- 1987 : Απολυτήριο 1ου Λυκείου Ηρακλείου, Βαθμός: 19⁶/₁₁
- Ιούνιος -Ιούλιος 1990 : Παρακολούθηση 1ου Θερινού Σχολείου Φυσικής του Πανεπιστημίου Κρήτης.
- Απρίλιος -Ιούλιος 1991 : University of Amsterdam, Astronomical Institute “Anton Pannekoek” . Εκπόνηση Διπλωματικής Εργασίας με θέμα : “*The two optical states in Scorpius X-1*”
- Σεπτέμβριος 1991 : Πτυχίο Φυσικής Πανεπιστημίου Κρήτης, Βαθμός:8.5
- 10/1991 - 1/1992: : Παρακολούθηση ειδικού κύκλου σεμιναρίων “ *Οι μικροεπεξεργαστές στις σύγχρονες διατάξεις ελέγχου και παραγωγής*” στο Τεχνολογικό Εκπαιδευτικό Ίδρυμα Ηρακλείου (Σχολή τεχνολογικών εφαρμογών) και εκπόνηση εργασίας με θέμα: “ *A/D Conversion, προγραμματισμός σε Pascal, γραφική απεικόνιση σε Προσωπικό Υπολογιστή και αποθήκευση σε σκληρό δίσκο* ”
- Φεβρουάριος 1992 : Εισαγωγή στο Μεταπτυχιακό Πρόγραμμα του Χημικού τμήματος Πανεπιστημίου Κρήτης.
- Νοέμβριος 1993 : Αποπεράτωση των υποχρεώσεων για λήψη Μεταπτυχιακού Διπλώματος Ειδίκευσης στη Φυσικοχημεία, και παρουσίαση Μεταπτυχιακής εργασίας με θέμα: “***Δυναμική Πολυσυσταδικών Πολυμερικών Συστημάτων Κοντά στο Σημείο Μετάβασης Τάξης***”
- Νοέμβριος 1993-Νοέμβριος 1997 : αμοιβόμενη εργασία στα πλαίσια ερευνητικών προγραμμάτων του Ιδρύματος Τεχνολογίας και Έρευνας
- Ιούλιος 1994 : Λήψη Μεταπτυχιακού Διπλώματος ειδίκευσης στη Φυσικοχημεία, με μέσο όρο στα μαθήματα 8.5
- Δεκέμβριος 1993 -Νοέμβριος 1997 : Εκπόνηση Διδακτορικής Διατριβής με τίτλο “***Δυναμική Συσταδικών Συμπολυμερών και Πολυμερικών Μειγμάτων: Διηλεκτρική Φασματοσκοπία και Προσομοιώσεις Monte Carlo .***”
Επιβλέποντες καθηγητές : Καθ. Γ. Φυτάς, Καθ. Σ. Αναστασιάδης
- Νοέμβριος 1997-Μάρτιος 2000 : Μεταδιδακτορικός ερευνητής στο Πανεπιστήμιο του Leeds (University of Leeds, Dept. of Physics and Astronomy and Interdisciplinary Research Center in Polymer Science and Technology).
Επιβλέποντες καθηγητές : Dr. D.B. Adolf, Prof. G.R.Davies
- Μάρτιος 2000-Ιούνιος 2001: Μεταδιδακτορικός ερευνητής στο Πανεπιστήμιο Βρυξελλών (Universite Libre de Bruxelles, Unite de Physique des Polymeres – CP223)
Επιβλέπων καθηγητής : Prof. Jean-Paul Ryckaert
- Ιούλιος 2001-Ιούλιος 2002 : Εκπλήρωση στρατιωτικών υποχρεώσεων
- Σεπτέμβριος 2002 – Φεβρουάριος 2003 : Διδάσκων (ΠΔ. 407, Βαθμίδα Αναπληρωτή Καθηγητή) στο τμήμα Επιστήμης και Τεχνολογίας Υλικών του Πανεπιστημίου Κρήτης
- Μάρτιος 2003-Απρίλιος 2008 : Λέκτορας του τμήματος Χημικών Μηχανικών του Αριστοτελείου Πανεπιστημίου Θεσσαλονίκης (Τομέας Χημείας, Εργαστήριο Φυσικής Χημείας).
- Απρίλιος 2008 - τώρα : Επίκουρος Καθηγητής του τμήματος Χημικών Μηχανικών του Αριστοτελείου Πανεπιστημίου Θεσσαλονίκης (Τομέας Χημείας, Εργαστήριο Φυσικής Χημείας).

Υποτροφίες

- Λήψη υποτροφίας από το Ι.Κ.Υ σε όλα τα έτη προπτυχιακών σπουδών.
- Υποτροφία Erasmus από Απρίλιο-Ιούλιο 1991
- 1992-1997 : Μεταπτυχιακός υπότροφος του Ιδρύματος Τεχνολογίας και Έρευνας Ινστιτούτο Ηλεκτρονικής Δομής και Laser.

Διδακτική πείρα:

- Βοηθός Εργαστηρίων Φυσικοχημείας για 2 έτη, Πανεπιστήμιο Κρήτης, Τμήμα Χημείας
- Επικουρικό διδακτικό έργο στο μάθημα της Φυσικοχημείας. για 1 έτος
- Σεπτέμβριος 2002-Φεβρουάριος 2003: Διδάσκων (ΠΔ 407 Βαθμίδα Αναπληρωτή Καθηγητή) στο μάθημα ΗΥ-0 (Εισαγωγή στους Η-Υ) του τμήματος Επιστήμης και Τεχνολογίας Υλικών Πανεπιστημίου Κρήτης.
- Οκτώβριος 2002 : Διδάσκων στο μάθημα Φυσικοχημεία-I του Χημικού τμήματος Πανεπιστημίου Κρήτης.
- Μάρτιος 2003 – τώρα : Πανεπιστήμιο Θεσσαλονίκης, Τμήμα Χημικών Μηχανικών, Εργαστήρια Φυσικοχημείας, Φυσικοχημεία Ι-Ασκήσεις
- Φεβρουάριος-Απρίλιος 2005, Απρίλιος 2011 : Διδάσκων στο μάθημα «Θερμοδυναμική και Κινητική των Υλικών» του Διατμηματικού Μεταπτυχιακού προγράμματος «Διεργασίες και Τεχνολογία Προηγμένων Υλικών», Αριστοτέλειο Πανεπιστήμιο Θεσσαλονίκης
- Οκτώβριος 2006 – τώρα : Πανεπιστήμιο Θεσσαλονίκης, Τμήμα Χημικών Μηχανικών , «Υπολογιστική Επιστήμη Υλικών»

Επίβλεψη φοιτητών

Διπλωματικές Εργασίες

Επιστημονικός Επιβλέπων

1. Βαβέκης Κωνσταντίνος , Πανεπιστήμιο Κρήτης, Τμήμα Χημείας, 1992
2. Βλάχος Γεώργιος, Πανεπιστήμιο Κρήτης, Τμήμα Χημείας, 1996
3. Κρυστάλλης Μάριος, Αριστοτέλειο Πανεπιστήμιο Θεσσαλονίκης, Τμ. Χημ. Μηχ., 2006
4. Λουφάκη Νέλλη, Αριστοτέλειο Πανεπιστήμιο Θεσσαλονίκης, Τμ. Χημ. Μηχ., 2009 (Συνεπίβλεψη με τον Καθ. Σ. Αναστασιάδη)
5. Ελευθερίου Ηλίας, Αριστοτέλειο Πανεπιστήμιο Θεσσαλονίκης, Τμ. Χημ. Μηχ., 2011

Συμμετοχή στην τριμελή εξεταστική επιτροπή των διπλωματικών εργασιών (Τμ. Χημ. Μηχανικών Α.Π.Θ.) των:

1. Κακκαλή Αθανάσιου
2. Αθανασίας Τσιμπλιάρη
3. Δαρδαγιαννοπούλου Άννας
4. Γεωργούλα Κων/νου
5. Τριανταφύλλου Απόστολου
6. Δρίτσα Γεώργιου
7. Σκούταρη Νικόλαου
8. Τσιόπτσια Κων/νου
9. Δημητρίου Ελένης
10. Κουτσόπουλου Κων/νου
11. Μέρκου Ιωάννη
12. Αγγελοπούλου Αναστασίας

13. Στυλιανού Χρυστάλλας
14. Παπαμιχαήλ Μαριάννας
15. Σωτηριάδου Αργυρώς
16. Φλώρου Στυλιανού
17. Χαλέβα Ελευθέριου
18. Κοκκινομάλλη Ιωάννη
19. Στεφόπουλου Απόστολου
20. Καραγεωργάκης Χρυσάνθης
21. Στουρνάρας Μαρίας-Ελευθερίας
22. Κράββας Μαρίας
23. Τατσούδης Δήμητρας
24. Ελ Αουρ Σαμι
25. Αισσα Γιανμά
26. Χατζηγεωργίου Προκόπη
27. Σπηλιώτη Αλέξιου
28. Φαίδωνος Σοφίας
29. Γαλλίκας Δέσποινας
30. Τασούλας Στυλιανής
31. Μιμίκου Νικολάου
32. Πλαχούρα Παναγιώτη
33. Χανδόλια Κωνταντίνου
34. Κυπριώτη Αναστασίου
35. Γαϊτανόπουλου Γεωργίου
36. Μινασίδη Βλαδίμηρου
37. Σαλλιακέλλη Παναγιώτη
38. Στεφανίδη Νικολάου
39. Σάββα Αχιλλέα
40. Ρούσσης Γεωργίας
41. Βαλοδήμου Κωνσταντίνας
42. Κοϊνη-Κυριακίδου Ίρις
43. Καλύβα Αγνή

Διατριβές για Μεταπτυχιακό Δίπλωμα Ειδίκευσης

Συμμετοχή στην τριμελή εξεταστική επιτροπή των

1. Κακκαλή Αθανάσιου Α.Π.Θ. , Διατμηματικό Πρόγραμμα Μεταπτ. Σπουδών, 2006
2. Αθανασίας Τσιμπλιάρη Α.Π.Θ. , Διατμηματικό Πρόγρ. Μεταπτ. Σπουδών, 2006
3. Δρίτσα Γεώργιου, Α.Π.Θ. , Διατμηματικό Πρόγραμμα Μεταπτ. Σπουδών, 2006
4. Καρκαντελίδου Φωτεινής , Α.Π.Θ. , Διατμηματικό Πρόγρ. Μεταπτ. Σπουδών, 2006
5. Κλάδη Κωνσταντίνας , Α.Π.Θ. , Διατμηματικό Πρόγραμμα Μεταπτ. Σπουδών, 2006
6. Παπανάνου Ελένης, Α.Π.Θ. , Διατμηματικό Πρόγραμμα Μεταπτ. Σπουδών, 2009

Επιβλέπων Μεταπτυχιακών Διπλωματικών Εργασιών

1. Συνεπιβλέπων της μεταπτυχιακής διπλωματικής εργασίας του Κ. Δημήτριου Τραγουδάρα, φοιτητή Διατμηματικού Προγρ. Μεταπτ. Σπουδών. «*Επιστήμη και Τεχνολογία Προηγμένων Υλικών*» (περάτωση Δεκέμβριος 2009)

2. Επιβλέπων της μεταπτυχιακής διπλωματικής εργασίας του Κ. Μάριου Κρυστάλλη, φοιτητή του Διατμηματικού Προγ. Μεταπτ. Σπουδών «*Νανοεπιστήμες και Νανοτεχνολογίες*», (περάτωση Οκτώβριος 2009)

Διδακτορικές Διατριβές

Συνυπεύθυνος επιστημονικός επιβλέπων στην διδακτορική εργασία του Κ. Stewart Hotston , Πανεπιστήμιο του Leeds, Τμήμα Φυσικής και Αστρονομίας, 1998-2002

Μέλος τριμελούς συμβουλευτικής επιτροπής των υποψηφίων διδακτόρων:

1. Κακκαλή Αθανάσιου – Α.Π.Θ. Τμ. Χημικών Μηχανικών, 2007-
2. Φλώρου Στυλιανού - Α.Π.Θ. Τμ. Χημικών Μηχανικών, 2010-

Κύριος Επιβλέπων Διδακτορικών διατριβών:

1. Τάνη Ιωάννη - Α.Π.Θ. Τμ. Χημ. Μηχανικών, 2005-2009
2. Δαλάκογλου Γεωγίου - Α.Π.Θ. Τμ. Χημ. Μηχανικών, 2005 –2009
3. Φωτιάδου Σαπφούς - Α.Π.Θ. Τμ. Χημ. Μηχανικών, 2008-

Μέλος της επταμελούς εξεταστικής επιτροπής των υποψηφίων διδακτόρων :

1. Παντούλας Μαρίας Α.Π.Θ. Τμ. Χημ. Μηχανικών Ιούλιος 2006
2. Μειμάρογλου Δημητρίου, Α.Π.Θ. Τμ. Χημ. Μηχανικών, Ιούλιος 2008
3. Δρίτσα Γεωργίου, Α.Π.Θ, Τμ. Χημικών Μηχανικών, Οκτώβριος 2009
4. Κουμάκη Νικολάου, Παν. Κρήτης, Τμ. Επιστ. κ Τεχν. Υλικών, Φεβρουάριος 2011
5. Μαντρούρλια Θεοφάνη, Α.Π.Θ., Τμ. Χημικών Μηχανικών, Ιούνιος 2011
6. Κοντογιαννόπουλος Κωνσταντίνος, Α.Π.Θ., Τμ. Χημικών Μηχανικών, Οκτώβριος 2011
7. Γεωργάκης Μιχαήλ, Τμ. Χημικών Μηχανικών, Απρίλιος 2012

Μέλος της 3μελούς εξεταστικής επιτροπής των υποψηφίων διδακτόρων
(Invited Extrenal Examiner, University of Trieste, April 2010)

1. Matteo Maria Dalmiglio
2. PAOLO LACOVIG
3. Barbara Lorenzut
4. GIOVANNI MARIA PAVAN
5. PAOLA POSOCCO
6. ANDREA TRAVAN
7. ANDREA UMERI

Διοικητική Πείρα

1. Συμμετοχή σε επιτροπές του τμήματος Χημικών Μηχανικών ΑΠΘ

- Επόπτης Κτιρίου Γ' της Πολυτεχνικής
- Επιτροπή Δημοσίων Σχέσεων, Σεμιναρίων, Εκδηλώσεων και Προβολής Τμήματος
- Επιτροπή Αξιολόγησης και Διασφάλισης Ποιότητας Σπουδών
- Επιτροπή κτιριακών υποδομών του Τομέα Χημείας
- Επιτροπή διεξαγωγής κατατακτηρίων εξετάσεων

2. Συμμετοχή σε επιτροπές της Κοσμητείας

- Επιτροπή εποπτικών κτιρίων της Πολυτεχνικής
- Επιτροπή για την εξέταση θεμάτων του Μετρώ
- Επιτροπή για την συλλογή στοιχείων του επετειακού τόμου των 50 ετών της Πολυτεχνικής

Επιπρόσθετη εμπειρία

Ξένες γλώσσες: Αγγλικά (άριστα), Γερμανικά (μέτρια)

Επισκέψεις με διαμονή σε Ιδρύματα του εξωτερικού:

- 4/1991-7/1991 University of Amsterdam, Astronomical Institute “Anton Pannekoek”, Amsterdam, The Netherlands
- 2/1994-3/1994 Max-Planck Institute fur PolymerForschung, Mainz, Germany
- 5/1995 National Institute of Standards and Technology, Washington DC, USA
- 6/1995 University of Leipzig, Leipzig, Germany
- 9/2000 Institute Laue-Langevin, Grenoble, France
- 12/2000 Heriot-Watt University, Edinburgh, Scotland, UK
- 9/2005 Technical University of Eindhoven, Applied Physics Department, Eindhoven, The Netherlands
- 1/2007 Center for Self Organization of Molecular Species (SOMS), Leeds, United Kingdom
- 2/2010-6/2010 University of Trieste, Department of Materials and Natural Resources, Chemical Engineering section (Sabbatical leave), Trieste, Italy

Τεχνικές-Υπολογιστικές Γνώσεις

Εμπειρία σε πειραματικές τεχνικές : Διηλεκτρική Φασματοσκοπία, Δυναμική Σκέδαση Φωτός, Διαφορική Θερμιδομετρία Σάρωσης (DSC), Σκέδαση νετρονίων

Εμπειρία στη χρήση λειτουργικών συστημάτων Ηλ. Υπολογιστών: Unix, Ms-Windows, Linux (εγκατάσταση και διαχείριση νησίδας υπολογιστών στο εργαστήριο Φυσικής Χημείας)

Εμπειρία στην χρήση πακέτων για προσομοιώσεις και υπολογισμούς : Materials Studio, DL_POLY, DL_PROTEIN, Mathematica

Γλώσσες Προγραμματισμού : C, FORTRAN, Pascal

Σχολεία : i) Como Summer School on Monte Carlo and Molecular Dynamics of condensed matter systems Como 1-31 July 1995,
ii) METHODS IN MOLECULAR SIMULATION CCP5/SMTG Spring School 25--31 March 1998, Bristol, UK
iii) Nato ASI School “Polymer & Colloid 99”, Advanced Study Institute, Les Houches, France, 14-24 September 1999

Επαγγελματικές Ενώσεις

Μέλος της *American Physical Society*

Μέλος της *Hellenic Polymer Society*

Δημοσιεύσεις

Δημοσιεύσεις σε Διεθνή Επιστημονικά Περιοδικά με κριτές (Refereed Journals)
(Διαθέσιμες και στην ιστοσελίδα <http://users.auth.gr/~kkaratas>)

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

J. 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

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
J. 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. **"Nanoscopic 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) (corresponding author)

13. **"Slow modes in local polymer dynamics"**

K. Karatasos and D. B. Adolf
J. Chem. Phys. (Communication) **112**(19), 8225,(2000) (corresponding author)

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 (Communication) **34**, 7232 (2001) (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)

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26. " **Effects of Topology and Size on Statics and Dynamics of Complexes of Hyperbranched Polymers with Linear Polyelectrolytes** "
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41. **Chimeric advanced drug delivery nano systems (chi-aDDnSs) for shikonin combining dendritic and liposomal technology**
 K. N. Kontogianopoulos, A. N. Assimopoulou, S. Hatziantoniou, K. Karatasos, C. Demetzos and V. P. Papageorgiou
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43. **Aspects of PAMAM-based Dendrimer/siRNA complexation as studied by computer simulations: effects of pH and generation on dendrimer structure and siRNA binding**
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H-Factor : 16 (Πηγή : ISI Web of Science+Scopus)

Στον υπολογισμό του h-factor υπεισέρχονται οι εξής δημοσιεύσεις (σε παρένθεση οι αναφορές από ISI Web of Science+Scopus, με έντονη γραμματοσειρά η σειρά κατάταξης)

1. 11 (195), **2.** 9 (84), **3.** 17 (77), **4.** 5 (49) , **5.** 10 (47), **6.** 3 (44), **7.** 6 (43), **8.** 4 (32), **9.** 19 (25) , **10.** 15 (20), **11.** 1 (18), **12.** 18 (17), **13.** 26 (17), **14.** 35 (17), **15.** 12 (16), **16.** 22 (16),

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17. K. Karatasos
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18. G.K. Dalakoglou, K. Karatasos, S. Lyulin, A. Lyulin
6th Panhellenic Chemical Engineering Scientific Conference Proceedings, Athens,
p. 1269, 2007
19. G.K. Dalakoglou, K. Karatasos, S. Lyulin, A. Lyulin
4th International Workshop on "Nanosciences & Nanotechnologies" (NN07)
July 2007, Thessaloniki, Greece, Abstract Book, pp 136, 2007
20. G.S. Dritsas, I. Tanis, K. Karatasos, C. Panayiotou
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21. K.Karatasos
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23. K. Karatasos, G. Dalakoglou, I. Tanis, M. Krystallis
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24. S. Lyulin, A. Lyulin, S. Larin, A. Darinskii, K. Karatasos
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25. G.K. Dalakoglou, K. Karatasos, S.V. Lyulin, A.V. Lyulin
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26. G.S. Dritsas, K. Karatasos, C. Panayiotou
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28. K. Karatasos
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1st International Conference “From Nanoparticles & Nanomaterials to Nanodevices
& Nanosystems”
Halkidiki, Greece, June 16-18, 2008
32. I.Tanis, K. Karatasos
7th Hellenic Polymer Conference, Ioannina, September 28th - October 1st 2008
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33. G. S. Dritsas, I. Tanis, M. Stournara, K. Karatasos, C. Panayiotou
7th Hellenic Polymer Conference, Ioannina, September 28th - October 1st 2008
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7th Panhellenic Scientific Conference in Chemical Engineering, Patras, 3-5 June 2009,

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36. K. Karatasos and I. Tanis,
6th International Dendrimer Symposium , Stockholm, June 14-18, 2009
Electronic Abstracts, page 98
37. S. Pricl, P. Posocco, M. Fermeglia, K. Karatasos, L. Peng and D. K. Smith
AIChE Annual Meeting, 2010, Salt Lake City, November 7-10, 2010
<http://aicheproceedings.org/2010/Fall/?page=15933> (607g)
38. S. Pricl, P. Posocco, E. Laurini, M. Fermeglia, K. Karatasos, L. Peng and D. K. Smith
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39. KOSTAS KARATASOS, SABRINA PRICL , PAOLA POSOCCO,ERIK LAURINI
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OCTOBER, 2010, BOOK OF ABSTRACTS, PAGE 15
40. K. Karatasos, P. Posocco, E. Laurini and S. Pricl
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Προσκεκλημένες ομιλίες

1. **"Segmental dynamics and morphology in phase separated binary polymer blends"**
DIELECTRICA 98, Monte de Caparica, Portugal, June 1998 (invited)
2. **"Short scale dynamics in Polyisobutylene"**
Eindhoven University of Technology, The Netherlands, June 2004 (invited)
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 (invited)*
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 (invited)
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 (Invited)*

8. Glass transition in "soft colloidal" systems: the dendrimer case*Workshop on "Colloidal Gels and Glasses", (invited)**Crete, Aldemar Knossos Royal Village, Hersonissos, 13/6/2008***9. "Molecular Dynamics of Dendrimers"***1st (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***8th 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)***Κριτής σε διεθνή περιοδικά / Προγράμματα****Κριτής Προγραμμάτων**

Peer Reviewer of the European Science Foundation (ESF)

Κριτής Διεθνών περιοδικών

1. Macromolecules

Αναγνώριση από το περιοδικό "Macromolecules" (IF 4.4) ως κριτή, στο 25% των κορυφαίων κριτών παγκοσμίως

2. Journal of Chemical Physics, (επίσης Τελικός Κριτής (adjudicator) Άρθρων)
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
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

Επιστημονικά Συνέδρια

Συμμετοχή σε επιτροπές συνεδρίων :

- προεδρεύων σε συνεδρία του 5^{ου} Πανελληνίου Επιστημονικού Συνεδρίου Χημικής Μηχανικής, Θεσσαλονίκη, Μάιος 2005
- προεδρεύων σε συνεδρία του 6th international symposium in Molecular Order and Mobility in Polymers, St. Petersburg, 2-6 June, 2008
- προεδρεύων σε συνεδρία του 6th international Dendrimer symposium , Stockholm June 14-18, 2009
- προεδρεύων σε συνεδρία του 7^{ου} Πανελληνίου Επιστημονικού Συνεδρίου Χημικής Μηχανικής, Πάτρα, 3-5 Ιουνίου 2009
- προεδρεύων σε συνεδρία του 8^{ου} Πανελληνίου Επιστημονικού Συνεδρίου Χημικής Μηχανικής, Θεσσαλονίκη, 26-28 Μαΐου 2011

Διοργάνωση Συνεδρίων/Σχολείων :

- Κύριος οργανωτής : *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 (Προϋπολογισμός 14000€ από ESF και 5000€ από το Υπουργείο Παιδείας και Θρησκευμάτων)
Web-site: <http://users.auth.gr/~kkaratas/workshop>
Organizers: K.Karatasos (principal), A.V.Lyulin
- Συνδιοργανωτής : 1st International Training School “*Computer Simulation Methods for Dendrimers*”, 12-10 April 2010, Eindhoven, The Netherlands
Organizers: A.V.Lyulin (principal), K.Karatasos (Προϋπολογισμός 40000€ χρηματοδότηση από ESF)
Web-site: <http://physlamp.phys.tue.nl/COST/>
- Μέλος της Οργανωτικής και της Επιστημονικής επιτροπής, στο International training school and workshop on “*Dendrimers as Composites of Advanced Drug Delivery nano-Systems (aDDnSs). Biomedical Applications*” October 3-7, 2011, Athens , Greece

Συμμετοχή σε επιστημονικά συνέδρια

1. G.Fytas, S.H Anastasiadis, K.Karatasos, and N. Hadjichristidis
“Segmental and Chain Dynamics in Disordered Diblock Copolymers”
13th General Conference of the Condensed Matter Division of the European Physical Society and The Deutsche Physicalische Gesellschaft, Μάρτιος 1993, Regensburg, Germany
2. K.Karatasos, S.H. Anastasiadis, G.Fytas, N.Hadjichristidis, and J.E.L Roovers
“Dielectric Chain Relaxation in Poly(styrene-b-isoprene) Diblock Copolymer Melts near The Order-Disorder Transition”
3rd International Discussion Meeting on Relaxation in Complex Systems, Ιούνιος 1993, Alicante, Spain
3. K.Karatasos, S.H. Anastasiadis, G.Fytas, N.Hadjichristidis, A.N Semenov, and J.E.L Roovers
“Dielectric Chain Relaxation in Poly(styrene-b-isoprene) Diblock Copolymer Melts near The Order-Disorder Transition”
6th International Symposium on Polymer Analysis and characterization, Ιούλιος 1993, Αγία Πελαγία Κρήτης, Ελλάδα
4. S.H. Anastasiadis, K.Karatasos, G.Fytas, S.Pispas, M.Pitsikalis, N.Hadjichristidis, A.N Semenov , J.E.L Roovers, and T. Pakula
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5. K.Karatasos, S.H. Anastasiadis, A.N Semenov, N.Hadjichristidis, G.Fytas, J.E.L Roovers, and T.Pakula
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General meeting 94, American Physical Society, Μόρτιος 1994, Pittsburgh, P.A.U.S.A. Bull. Amer. Phys. Soc. 39,696 (1994)
6. K.Karatasos, S.H. Anastasiadis, G.Fytas, and T.Pakula
“Computer Simulation of the Static and Dynamic Behavior of Diblock Copolymers near The Ordering Transition”
General Meeting 95, American Physical Society, Μάρτιος 1995, San Jose, C.A, U.S.A, Bull. Amer. Phys. Soc. 40, 1995
7. G.Fytas, K.Karatasos, S.H. Anastasiadis, D. Vlassopoulos, G. Floudas, A.N. Semenov, S Pispas, M.Pitsikalis, N.Hadjichristidis, H.Watanabe, and T.Pakula
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General Meeting 95, American Physical Society, Μάρτιος 1995, San Jose, C.A, U.S.A, Bull. Amer. Phys. Soc. 40, 1995
8. T.Jian, K.Karatasos, S.H. Anastasiadis, G.Fytas, K. Chrissopoulou, K. Adamczyk, A.N. Semenov, S.Pispas, M.Pitsikalis, N.Hadjichristidis, and J.E.L Roovers
“Relaxation of Composition Fluctuations in Diblock Copolymer Melts near the Order-Disorder Transition Investigated by Polarized Dynamic Light Scattering”

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“Effect of Concentration Fluctuations on the Segmental Relaxation in homogeneous diblocks PIP-b-PVE”
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12. K.Karatasos, S.H Anastasiadis, F.Kremer, H. Watanabe
"Determination of Loops to Bridges Ratio in Triblock Copolymers by Dielectric Spectroscopy"
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13. K.Karatasos, S.H Anastasiadis, F.Kremer, H. Watanabe
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14. K. Karatasos, Spiros H. Anastasiadis, George Fytas Sanat K. Kumar, Ralph H. Colby
"Concentration Fluctuation Induced Dynamic Heterogeneities in Polymer Blends"
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15. K. Karatasos , S.H Anastasiadis, H.Watanabe, T. Pakula
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16. K. Karatasos, S.H. Anastasiadis, F. Kremer, H.Watanabe, T. Pakula
"On the Loops to Bridges Ratio in Ordered Triblock Copolymer Melts"
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17. D. Vlassopoulos, K. Karatasos, G. Fytas, T. Pakula and J. Roovers
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67th Annual Meeting of the Society of Rheology, Galveston, TX, February 1997

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"Dielectric Studies on the Dynamics of Phase Separated Binary Polymer Blends"
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"Dynamics of Multiarm Star Polymers in the Ordering Region" invited
3rd International Discussion on Relaxations in Complex Systems, Vigo, Spain June 30- July 11, 1997
21. K. Karatasos, S. H. Anastasiadis, G. Vlachos, E. Manias and E. P. Giannelis
"Effects of confinement on the segmental dynamics"
General Meeting 1998, APS, Los Angeles, March 1998
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Workshop, DIELECTRICA 98, Monte de Caparica, Portugal, June 1998
23. S. H. Anastasiadis, K. Karatasos, G. Vlachos, E. Manias, and E. P. Giannelis
"Confinement Effects on the Local Motion in nanocomposites"
1998 Fall Meeting of the Materials Research Society, December 1998, Boston, MA, U.S.A.
24. K. Karatasos, G. Floudas, G. Fytas, S. Kamath, R. H. Golby, S. K. Kamath and J. E. L. Roovers
"Component dynamics of miscible polymer blends : comparison of the predictions of a concentration fluctuation model to experiment"
Polymer & Colloid 99, Advanced Study Institute, Les Houches, France, 1999
25. K. Karatasos, S. H. Anastasiadis, T. Pakula and H. Watanabe
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27. S. Hotston, K. Karatasos, and D. B. Adolf
"Effects of pressure and temperature on the static and dynamic properties via NPT Molecular Dynamics Simulations"
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28. S. H. Anastasiadis, K. Karatasos, G. Vlachos, E. Manias and E. P. Giannelis
"Local Dynamics Under Severe Confinement in Nanocomposites "
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"Local Dynamics in PIB and aPP melts: Molecular Dynamics Simulations vs Experiment"
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- 30., G. Ariedi and K. Karatasos

“On the use of conic constraints to freeze hydrogen vibrations in full atomic simulations of polymers: local dynamics of Polypropylene and Polyisobutylene.”
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31. K. Chrissopoulou, S. H. Anastasiadis, R. Krishnamoorti, K. Karatasos, G. Vlachos, E. Manias and E. P. Giannelis
"Polymer Dynamics under Nanoscopic Confinement"
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32. K. Karatasos and J.-P. Ryckaert
"Local dynamics of polyisobutylene revisited"
Belgian Polymer Group, General Meeting 2001, 16-17 March, Sunparks Mol, Belgium
33. K. Karatasos, and D.B. Adolf
“Effect of Density on Local Segmental Polymer Dynamics: A Molecular Dynamics Study “
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34. 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
35. 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
36. K. Karatasos and J.-P. Ryckaert
4th International Discussion Meeting on Relaxations in Complex Systems
"Methyl dynamics and β -relaxation in polyisobutylene as studied by molecular dynamics simulations"
June 17-24 2001, Hersonissos, Crete, Greece
37. 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”
38. K. Chrissopoulou, 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”
39. 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"

40. K. Karatasos, J-P. Ryckaert
Jülich Soft Matter Days 19 - 22 November 2002, Kerkrade, NL
41. Kahle, S.; Monkenbusch, M.; Richter, D.; Ryckaert, J. P.; Karatasos, K.; Koza, M.
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43. K. Chrissopoulou, 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
44. K. Karatasos, D. B. Adolf and G. Davies
"Static and dynamic properties of model dendrimers"
3rd Chemical Engineering Conference for Collaborative Research in Eastern Mediterranean, 13-15 May 2003, Sani, Chalkidiki
45. K. Chrissopoulou, K. Karatasos, S. H. Anastasiadis, E. P. Giannelis, B. Frick
« **Effects of strong spatial confinement in polymer chain dynamics** »
4th Hellenic conference in Chemical Engineering, Patras, May 2003
46. Μαρράς Σ., Ζουμπουρτικούδης Ι., Καρατάσος Κ., Σικαλίδης Κ. και Παναγιώτου Κ.
ΑΝΑΠΤΥΞΗ ΝΕΩΝ ΝΑΝΟΣΥΝΘΕΩΝ ΒΙΟΑΠΟΙΚΟΔΟΜΗΣΙΜΩΝ ΚΑΙ ΒΙΟΣΥΜΒΑΤΩΝ ΠΟΛΥΜΕΡΙΚΩΝ ΥΛΙΚΩΝ ΜΕ ΟΡΥΚΤΑ ΤΗΣ ΑΡΓΙΛΟΥ
XX Πανελλήνιο συνέδριο Φυσικής Στερεάς Κατάστασης-Επιστήμης Υλικών
Ιωάννινα, Σεπτέμβριος 2004
47. 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 2004, Phodes, Greece
(Conference Proceedings, Vol 1/2 , p. 81)
48. JP Ryckaert, G. Ariedi, K. Karatasos
"Local Dynamics in Polymer Melts : From Individual Jumps to Diffusive Coarse-Grained Dynamics" (Invited)
Conference on Computational Physics 2004 Genoa Italy, 1-4 September 2004
49. Ryckaert, J.-P., Ariedi G. , Karatasos K.
"From local dynamics to conformational diffusion in polymer melts well above Tg"
N2M2 Neutron and Numerical Methods 2, Institute Laue Langevin, September 2004, Grenoble, France (invited)
50. K. Karatasos
"Statics and dynamics in model dendrimer melts: toward the glass transition"
5th Panhellenic Scientific Conference in Chemical Engineering

Thessaloniki, May 26-28 2005, Greece

51. 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)*

52. K. Karatasos
"Statics and Dynamics in Model Dendrimer Melts"
 2006 APS March Meeting, March 13-17, Baltimore, Maryland, U.S.A.

53. AERC 2006, Third Annual European Rheology Conference, April 27-29, Hersonissos, Crete, 2006

54. 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 (*invited*)

55. K. Karatasos
"Glassy Behavior in Nanoscale Dendritic Polymers"
3rd Workshop on Nanoscience & Nanotechnologies (N&N06), 10-12 July, 2006, Thessaloniki, Greece

56. K. Karatasos
"Local Scale Dynamics in Model Dendrimer Melts"
 6th Hellenic Conference on Polymers, Patras, 3-5 November 2006

57. G.K. Dalakoglou, K. Karatasos, S. Lyulin, A. Lyulin
"Brownian Dynamics Simulations of Complexes of HYperbranched Polymers with Linear Polyelectrolytes"
 6th Panhellenic Chemical Engineering Scientific Conference, Athens, May 2007

58. K. Karatasos
"Controlling Self Organization in Dendrimer Polyelectrolytes"
 HPC-Europa, Fourth Translational Access and Mobility Workshop (TAM '07), Bolonia, Italy, June 13-15, 2007 (*invited*)

59. 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), Bolonia, Italy, June 13-15, 2007

60. 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

61. 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”
1st 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
66. 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
67. G.S. Dritisas, 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
68. 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
69. 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.
70. 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.
71. 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

72. G. K. Dalakoglou, K. Karatasos, S.V. Lyulin, A.V. Lyulin
Modelling of Complexes of Hyperbranched Polymers with Linear Polyelectrolytes in Shear Flows
5th International Conference on Nanosciences and Nanotechnologies (N&N08)
Thessaloniki 14-16 July 2008 ,
73. K. Karatasos and M. Krystallis
Self-Ordering in Model Dendrimer Polyelectrolytes
1st International Conference “From Nanoparticles & Nanomaterials to Nanodevices & Nanosystems”
Halkidiki, Greece, June 16-18, 2008
74. 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
75. 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
76. 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
77. Karatasos and M. Krystallis
STATICS AND DYNAMICS IN COULOMBIC-DRIVEN ORDERING IN MODEL DENDRIMER POLYELECTROLYTES: A MOLECULAR DYNAMICS SIMULATION STUDY
7th Panhellenic Chemical Engineering Scientific Conference, Patras, 3-5 June 2009
78. K. Karatasos and I. Tanis
Complexes of Poly(amidoamine) dendrimers in aqueous solutions as studied by molecular dynamics simulations
6th International Dendrimer Symposium 2009, Stockholm, Sweden, 14-18 June 2009
79. KOSTAS KARATASOS, SABRINA PRICL , PAOLA POSOCCO,ERIK LAURINI
A MOLECULAR DYNAMICS SIMULATION STUDY ON SI-RNA/TEA-PAMAM DENDRIMER COMPLEXATION
8TH HELLENIC POLYMER SOCIETY SYMPOSIUM , HERONISSOS CRETE, 24 – 29 OCTOBER, 2010
80. S. 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

<http://aicheproceedings.org/2010/Fall/?page=15933> (607g)

81. 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
82. 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
83. K. Karatasos
Modeling Hyperbranched Polymers for Drug and Gene Delivery Applications
 8th International Conference on Nanosciences & Nanotechnologies 12-15 July,
 Thessaloniki, Greece

Συμμετοχή σε επιστημονικά προγράμματα**Συμμετοχή σε διεθνή επιστημονικά προγράμματα συνεργασίας**

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. Πρόγραμμα COST της European Science Foundation (Network) “**Biomedical applications of Dendrimers**” (2009-2013) (Εκπρόσωπος της Ελλάδας στο Management Committee)

Συμμετοχή σε άλλα επιστημονικά προγράμματα

1. Μικροπορώδη Σύνθετα Υλικά Βιοπολυμερών – Υδροξυαπατίτη για την Κατασκευή Υποκατάστατων Οστών και την Ελεγχόμενη Απελευθέρωση Φαρμακευτικών Ουσιών. ΥΠΕΠΘ, ΠΥΘΑΓΟΡΑΣ Ι 2004
2. Μελέτη Νανοσυστημάτων Υπερδιακλαδισμένων Πολυμερών και Συμπλεγμάτων τους με Πολυηλεκτρολύτες, ως Παράγοντες Ενίσχυσης της Διαλυτότητας και Οχήματα Ελεγχόμενης Δέσμευσης/Αποδέσμευσης Φαρμάκων ή Βιοϋλικών. ΠΕΝΕΔ 2003, ΓΓΕΤ, 2005-2008 (ΕΠΙΣΤΗΜΟΝΙΚΟΣ ΥΠΕΥΘΥΝΟΣ, Προϋπολογισμός 198000€)
3. Χρηματοδότηση από το Υπουργείο Παιδείας και Θρησκευμάτων (2008) ποσού 5000€ για τη διοργάνωση διεθνούς συνεδρίου συνεργασίας (HYPER-NANO 2008)

4. 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) (ΠΡΟΣΩΠΙΚΗ ΕΠΙΧΟΡΗΓΗΣΗ)

5. 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) (ΠΡΟΣΩΠΙΚΗ ΕΠΙΧΟΡΗΓΗΣΗ)

6. HPC-Europa 2 project, funded by the European Commission - DG Research in the 7th 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**” (ΠΡΟΣΩΠΙΚΗ ΕΠΙΧΟΡΗΓΗΣΗ)

Συμμετοχή στη συγγραφή επιστημονικών προγραμμάτων που δεν χρηματοδοτήθηκαν η βρίσκονται στο στάδιο της κρίσης

1. “*Amphiphilic and Liquid crystal formulation Engineering through Rheologic and Thermodynamic properties*” FP7-NMP-2007-SMALL-1 (προήχθει στη Β φάση, δεν χρηματοδοτήθηκε)
2. “*A new system for developing efficacious tumour-targeted nanoparticles and its biological and industrial validation: integration of multidisciplinary methods*” FP7-NMP-2009-SMALL-3 (δεν χρηματοδοτήθηκε)
3. “*Separation of branched polymers*” (SeBra) FP7-PEOPLE-ITN-2008 (προήχθει στη Β φάση, δεν χρηματοδοτήθηκε)
4. “*Multifunctional Complexes of Hyperbranched Polyelectrolytes with Surfactants: Role of Chemical Structure and Thermodynamic Environment*” DPI-CRP (αρχικώς εγκρίθηκε, η χρηματοδότηση δεν πραγματοποιήθηκε λόγω απόσυρσης της εταιρείας DSM)
5. “*Development and evaluation of nanocarriers based on hyperbranched polymers , for pharmaceutical/biomedical uses: from molecular design to application*” “THALIS” ΕΣΠΑ 2010-2013 (coordinator, δεν χρηματοδοτήθηκε)
6. “*High performance nanocomposite materials: Reinforcement of polymers with advanced carbon and silica nanostructures*” “THALIS” ΕΣΠΑ 2010-2013 (προήχθει στη Β φάση, αναμένεται τελική έγκριση)
7. “*Study of the Self-Assembly of Hyperbranched Polymers on Surfaces*” 2011, Latsis Foundation (στη διαδικασία κρίσης)

Αναφορές

Ειδικές Αναφορές

1. Η εργασία

"Composition Fluctuation Effects on Dielectric Normal Mode Relaxation in Diblock Copolymers. II Disordered State in the proximity to the ODT and Ordered State"
Macromolecules **29**, 1326 (1996)

αναφέρεται στο βιβλίο “*Block Copolymers: Synthetic Strategies, Physical Properties, and Applications*” των N. Hadjichristidis, S. Pispas and G. Floudas, Wiley Interscience 2003 όπου Karatasos K.

παρουσιάζεται εικόνα (Fig. 20.9) βασισμένη στα αποτελέσματα της παραπάνω εργασίας, ενώ αναφέρεται και στο βιβλίο “*Simulation Methods for Polymers*” (M. Kotelyanskii and D. N. Theodorou Eds, Dekker, New York 2004) (αναφορά 41, Κεφ. 5)

2. Η εργασία

"Statics and Dynamics of model dendrimers as studied by molecular dynamics simulations"

J. Chem. Phys. **115**,5310 (2001)

αναφέρεται στο άρθρο ανασκόπησης (Review) Pethrick RA “**Molecular motion in polymer systems**” CURR OPIN SOLID ST M 6 (3): 221-225 JUN 2002 και χαρακτηρίζεται ως “*of outstanding interest*” για το συγκεκριμένο ερευνητικό πεδίο

Αναφέρεται επίσης ως μια από τις εξέχουσες εργασίες στο πεδίο των μοριακών προσομοιώσεων των δενδριμερών, στο βιβλίο “**Dendrimer-Based Nanomedicine**” (ed. I. J. Majoros and J. R. Baker JR, Pan Stanford Publishing: Singapore, 2008;) σελ 334.

3. Ειδική μνεία γίνεται για τις εργασίες

"Effects of density on the local dynamics and conformational statistics in polyethylene: a Molecular Dynamics Study"

J. Chem. Phys. (2000) **112**(19), 8695, (2000)

"Slow modes in local polymer dynamics"

J. Chem. Phys. (Communication) **112**(19), 8225,(2000)

από το άρθρο ανασκόπησης *Molecular Simulation*, 2002 Vol. **28** (5), pp. 385–471 των W. SMITH, C.W. YONG and P.M. RODGER , όπου αφιερώνονται 4 σελίδες στην περιγραφή των αποτελεσμάτων των εργασιών αυτών (δείχνεται αυτούσια εικόνα , η Fig. 5.) ενώ σημειώνεται

“*Overall the work of Karatasos et al. represents a revealing example of what MD can provide in understanding molecular processes.*”

4. Για την απήχηση της εργασίας

"Nanoscale confinement effects on local dynamics"

Phys. Rev. Lett., **84**(5), 915 (2000)

έγινε ειδική αναφορά από το Science Citation Index σημειώνοντας

“*..the number of citations your article received places it in the top 1% within its field according to Essential Science Indicators. Your work is highly influential, and is making a significant impact among your colleagues in your field of study*”

ενώ αφιερώνεται και ειδική παράγραφος στο βιβλίο “*Physical Properties of Polymers*” page 75, Cambridge University Press, 2003

5. Η εργασία

Computer simulation of static and dynamic behavior of diblock copolymer melts

Pakula T, Karatasos K, Anastasiadis SH, Fytas G

αναφέρεται εκτενώς στο Κεφ. 5 “*Simulations on the completely occupied Lattice*” στην παράγραφο “**C. Block Copolymers**” (σελ 175) του βιβλίου “*Simulation Methods for Polymers*” (M. Kotelyanskii and D. N. Theodorou Eds, Dekker, New York 2004) (αναφορά 38) , όπου και δείχνεται η εικόνα 1 της εργασίας (εικ. 6 του Κεφαλαίου) καθώς και μέρος της εικόνας 6 της εργασίας (εικ. 7 του Κεφαλαίου)

6. Η εργασία

On the loops-to-bridges ratio in ordered triblock copolymers: An investigation by dielectric relaxation spectroscopy and computer simulations

Karatasos K, Anastasiadis SH, Pakula T, et al.

MACROMOLECULES 33 (2): 523-541 JAN 25 2000

αναφέρεται επανειλημμένα στο βιβλίο “*Development in Block Copolymer Science and Technology*” (John Wiley & Sons, 2004, I. Hamley) ενώ κάποια από τα αποτελέσματα αυτής παρουσιάζονται ως τα πλέον αποδεκτά

5. Η εργασία

"Non-Gaussian nature of Glassy Dynamics by Cage-to-Cage Motion"

B. Vorselaars, A.V. Lyulin, K. Karatasos and M. A. J. Michels

Physical Review E **75**, 011504 (2007)

επιλέχθηκε να εμφανιστεί στο ηλεκτρονικό περιοδικό *Virtual Journal of Biological Physics Research* στον τομέα **FUNDAMENTAL POLYMER STATICS/DYNAMICS**. Παρατίθεται μέρος από την ηλεκτρονική επιστολή του εκδότη :

«We are pleased to inform you that your article, "Non-Gaussian nature of glassy dynamics by cage to cage motion," published in *Physical Review E* 75, 011504 (2007), has been selected for the February 1, 2007 issue of **Virtual Journal of Biological Physics Research**. The Virtual Journal, which is published by the American Physical Society and the American Institute of Physics in cooperation with numerous other societies and publishers, is an edited compilation of links to articles from..»

6. Η εργασία “**Effects of Topology and Size on Statics and Dynamics of Complexes of Hyperbranched Polymers with Linear Polyelectrolytes**”

Journal of Chemical Physics, Art. No. 214903 (2007)

G. K. Dalakoglou, K. Karatasos, S.V.Lyulin, A.V.Lyulin

Επιλέχθηκε για επαναδημοσίευση σε 2 ηλεκτρονικά περιοδικά

A) «We are pleased to inform you that your article, "Effects of topology and size on statics and dynamics of complexes of hyperbranched polymers with linear polyelectrolytes," published in *The Journal of Chemical Physics* 127, 214903 (2007), has been selected for the December 24, 2007 issue of **Virtual Journal of Nanoscale Science & Technology**. The Virtual Journal, which is published by the American Institute of Physics and the American Physical Society in cooperation with numerous other societies and publishers, is an edited compilation of links to articles from participating publishers, covering a focused area of frontier research. You can access the Virtual Journal at <http://www.vjnano.org> – thank you for your contribution.»

B) «We are pleased to inform you that your article, "Effects of topology and size on statics and dynamics of complexes of hyperbranched polymers with linear polyelectrolytes," published in *The Journal of Chemical Physics* 127, 214903 (2007), has been selected for the December 15, 2007 issue of **Virtual Journal of Biological Physics Research**. The Virtual Journal, which is published by the American Physical Society and the American Institute of Physics in cooperation with numerous other societies and publishers, is an edited compilation of links to articles from participating publishers, covering a focused area of frontier research. You can access the Virtual Journal at <http://www.vjbio.org> -- thank you for your contribution.»

7. Τα αποτελέσματα της συνεργασίας σε πανευρωπαϊκό επίπεδο στα πλαίσια του συνεδρίου εργασίας HYPER-NANO 2008 (Κ. Καρατάσος, Κύριος οργανωτής) αποτέλεσαν ειδική δημοσίευση στην ιστοσελίδα της European Science Foundation www.esf.org. (24 Οκτωβρίου 2008) με τίτλο «*New molecules with many branches will help unleash potential of nanotechnology*» το οποίο αναδημοσιεύτηκε σε πολλές επιστημονικές ιστοσελίδες με θέμα την νανοτεχνολογία

([http://www.esf.org/research-areas/physical-and-engineering-sciences/news/ext-news-singleview.html?tx_ttnews\[pointer\]=1&tx_ttnews\[tt_news\]=510&tx_ttnews\[backPid\]=28&cash=6861dc8f5c](http://www.esf.org/research-areas/physical-and-engineering-sciences/news/ext-news-singleview.html?tx_ttnews[pointer]=1&tx_ttnews[tt_news]=510&tx_ttnews[backPid]=28&cash=6861dc8f5c))

8. Το HYPER-NANO 2008 επιλέχθηκε ανάμεσα από όλα τα άλλα Exploratory Workshops που χρηματοδοτήθηκαν από την ESF (τυπικά 50 κάθε χρόνο σε όλη την Ευρώπη), για να περιληφθεί στην έκδοση των “ESF-Highlights-2008” στην οποία τονίζεται η σπουδαιότητα των συμπερασμάτων του σε Πανευρωπαϊκό επίπεδο.

http://www.esf.org/index.php?eID=tx_nawsecured1&u=0&file=fileadmin/be_user/research_areas/PESC/Documents/Highlights/Highlights-08.pdf&t=1302691496&hash=781f4d495a5d85fd4c108aa926e2fc

9. Η εργασία “**Dynamics of counterions in Dendrimer Polyelectrolyte Solutions**”

K. Karatasos and M. Krystallis

Journal of Chemical Physics **2009**, 130, 114903

επιλέχθηκε για αναδημοσίευση στο περιοδικό *Virtual Journal of Biological Physics Research* “We are pleased to inform you that your article, “Dynamics of counterions in dendrimer polyelectrolyte solutions,” published in *The Journal of Chemical Physics* 130, 114903 (2009), has been selected for the April 1, 2009 issue of *Virtual Journal of Biological Physics Research*. The *Virtual Journal*, which is published by the American Physical Society and the American Institute of Physics in cooperation with numerous other societies and publishers, is an edited compilation of links to articles from participating publishers, covering a focused area of frontier research. You can access the *Virtual Journal* at <http://www.vjbio.org> -- thank you for your contribution”

Αριθμός αναφορών από βιβλία (Πηγές : books.google.com, September 2011) : 45

Αριθμός αναφορών από άρθρα περιοδικών (Πηγές : ISI Web of Science, Scopus)

Συνολικός αριθμός αναφορών (citations) από περιοδικά (τελευταία ενημέρωση 2/’12) : 921

Συνολικός αριθμός ετεροαναφορών (non-self citations) από περιοδικά : 820

Πίνακας με τους παράγοντες απήγησης των περιοδικών όπου έγιναν οι δημοσιεύσεις

Περιοδικό	Παράγοντας απήγησης (2010)	Αριθμός δημοσιεύσεων
Astron. & Astrophysics	4.410	1
J. Chem. Phys.	2.920	10
Macromolecules	4.837	13
Macr. Th. Simulation	1.440	1
Molecular Simulation	1.215	1
Europhysics Letters	2.753	1
Physical Review E	2.352	1
Physical Review Letters	7.621	1
Physica B	0.856	1
Soft Matter	4.457	1

Materials Science & Eng. B.	1.560	1
Journal of Polymer Science Part B: Polymer Physics	1.298	1
Physica Scripta	0.982	1
Macromolecular Symposia	0.913 (IF. 2006)	1
Physical Chemistry Chemical Physics	3.453	2
Journal of Chromatography A	4.194	1
Journal of Physical Chemistry B	3.603	2
Macromolecular Bioscience	3.458	1
International Journal of Pharmaceutics	3.607	1
Polymers	(New Journal)	1

Αναλυτική παράθεση αναφορών ανά άρθρο σε περιοδικά με κριτή (-ές)

➤ ***COORDINATED X-RAY AND OPTICAL OBSERVATIONS OF SCORPIUS X-1***
 AUGUSTEIJN T, KARATASOS K, PAPADAKIS M, PATERAKIS G, KIKUCHI S,
 BROSCHE N, LEIBOWITZ E, HERTZ P, MITSUDA K, DOTANI T, LEWIN WHG,
 VANDERKLIS M, VANPARADIJS J
ASTRONOMY AND ASTROPHYSICS
 265 (1): 177-182 NOV 1992

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ASTROPHYS J 568 (2): 878-900 Part 1 APR 1 2002

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MON NOT R ASTRON SOC 311 (1): 201-224 JAN 1 2000

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TOTAL CITATIONS : 18

NON-SELF CITATIONS : 18

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➤ **LOCAL AND GLOBAL CHAIN DYNAMICS IN DIBLOCK COPOLYMER
MELTS**

FYTAS G, ANASTASIADIS SH, KARATASOS K, HADJICHRISTIDIS N
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**COMPOSITION FLUCTUATION EFFECTS ON DIELECTRIC NORMAL-
MODE RELAXATION IN DIBLOCK COPOLYMERS .1. WEAK
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2. ANASTASIADIS SH, JIAN T, FYTAS G
**DYNAMIC LIGHT-SCATTERING FROM DIBLOCK COPOLYMER
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NON-SELF CITATIONS : 11

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➤ KARATASOS K, ANASTASIADIS SH, SEMENOV AN, et al.
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DYNAMICS OF COMPOSITION FLUCTUATIONS IN DIBLOCK COPOLYMER SOLUTIONS FAR FROM AND NEAR TO THE ORDERING TRANSITION
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MOL PHYS 96 (2): 149-160 JAN 20 1999
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Phys. Chem. Chem. Phys., 1999, 1, 3923-3931
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Diblock copolymer dynamics
CURR OPIN COLLOID IN 5 (5-6): 324-333 NOV 2000

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Relaxation time distribution from time and frequency domain dielectric spectroscopy in poly(aryl ether ether ketone)
J CHEM PHYS 113 (2): 863-868 JUL 8 2000
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Nanoscale-confinement effects on local dynamics
PHYS REV LETT 84 (5): 915-918 JAN 31 2000
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Dielectric and dynamic mechanical relaxations in polymer-heterocycle hybrid materials
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Self-Concentration and Interfacial Fluctuation Effects on the Local Segmental Dynamics of Nanostructured Diblock Copolymer Melts
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 Macromolecules; **2010**; 43 pp 5740
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Journal of Materials Chemistry, 20, pp 9484, **2010**
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TOTAL CITATIONS : 44

NON-SELF CITATIONS : 37

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➤ **Composition fluctuation effects on dielectric normal-mode relaxation in diblock copolymers .2. Disordered state in proximity to the ODT and ordered state**

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➤ **Segmental dynamics of miscible polymer blends: Comparison of the predictions of a concentration fluctuation model to experiment**

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Συνοπτικό υπόμνημα των δημοσιευμένων ερευνητικών εργασιών

Περιγραφή της ερευνητικής εργασίας στα πλαίσια της Διδακτορικής Διατριβής

Τα κύρια σημεία συνεισφοράς της διατριβής αφορούν την κατανόηση της σχέσης Δυναμική-Θερμοδυναμική κατάσταση-Μορφολογία σε ορισμένες κατηγορίες συσταδικών συμπολυμερών (copolymers), πολυμερικών μειγμάτων (blends), και συνθέτων (composites). Επίσης μελετήθηκε η δυναμική και τα μορφολογικά χαρακτηριστικά πολυμερικών υλικών ειδικού τύπου (αστεροειδή) στην κατάσταση τήγματος.

Παρακάτω δίνονται λεπτομέρειες για τις επί μέρους θεματικές ενότητες στις οποίες μπορεί να χωριστεί η διατριβή

A) Συσταδικά συμπολυμερή

Περιγράφηκε η δυναμική συμπεριφορά στα τήγματα δυσσταδικών συμπολυμερών σε μια ευρεία περιοχή της θερμοδυναμικής τους κατάστασης. Η ομογενής περιοχή, περιγράφηκε παίρνοντας υπόψη τις διακυμάνσεις στη σύσταση τόσο εξαιτίας της προσέγγισης στην περιοχή Μετάβασης Τάξης-Αταξίας (ODT), όσο και λόγω της διαφοράς στην τοπική δυναμική των συστατικών τους. Στην περιοχή κοντά στην μετάβαση τάξης, αλλά και μετά τον μικροφασικό διαχωρισμό, παρατηρήθηκαν και αναγνωρίστηκαν νέοι τρόποι χαλάρωσης στην δυναμική των αλυσίδων, ενώ δείχτηκε και η αλληλοεξάρτηση των χαρακτηριστικών της δυναμικής από τα ειδικά μορφολογικά χαρακτηριστικά της σχηματιζόμενης μικροδομής, στην κατάσταση τάξης. Για την ανάλυση των συχνά πολύπλοκων φασμάτων, αναπτύχθηκε μια νέα μεθοδολογία μέσω της οποίας κατέστη δυνατός ο υπολογισμός της κατανομής των χαρακτηριστικών τρόπων χαλάρωσης, παρακάμπτοντας έτσι την επιστράτευση καθαρά εμπειρικών (και συχνά ανεπαρκών) παλαιότερων μεθόδων.

Μέσω προσομοιώσεων Monte Carlo με τον αλγόριθμο CMA (Cooperative Motion Algorithm), έγινε η συστηματική μελέτη στατικών και δυναμικών ιδιοτήτων μοντέλων δυσσταδικών συμπολυμερών, σε ολόκληρη την θερμοδυναμική περιοχή στην κατάσταση τήγματος, τα αποτελέσματα της οποίας συγκρίθηκαν με επιτυχία με τα πειράματα.

Σχετικές δημοσιεύσεις. :

- **"Local and Global Chain Dynamics in Diblock Copolymer Melts"**

G. Fytas, S.H. Anastasiadis, K. Karatasos, and N. Hadjichristidis

Physica Scripta, **T49**, 237 (1993)

- **"Composition Fluctuation effects on Dielectric Normal Mode Relaxation in Diblock**

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Copolymers. I Weak Segregation Regime"

K. Karatasos, S. H. Anastasiadis, G.Fytas, A. N. Semenov, M. Pitsikalis, and N. Hadjichristidis

Macromolecules **27**, 3543 (1994)

- **"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)
- **"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)

Στο πλαίσιο της προσπάθειας για την εξαγωγή πληροφορίας σχετιζόμενης με τα μορφολογικά χαρακτηριστικά στην κατάσταση τάξης από δυναμικές μελέτες, εξετάστηκε ένα ειδικά για τον σκοπό αυτό κατασκευασμένο σύστημα, συμμετρικού τρισυσταδικού συμπολυμερούς σε συνδυασμό με το ομόλογο δισυσταδικό συμπολυμερές του, τόσο πειραματικά όσο και με Monte Carlo (CMA) προσομοιώσεις. Ερευνήθηκε η σχέση των χαρακτηριστικών της μικροδομής (φυλλώδης δομή στην συγκεκριμένη περίπτωση) και των διαφορετικών διαμορφώσεων (βρόγχοι ή γέφυρες) στην δυναμική των αλυσίδων, ενώ έγινε και υπολογισμός του (σημαντικού στον καθορισμό πολλών μακροσκοπικών ιδιοτήτων) σχετικού ποσοστού των γεφυρών και βρόγχων, με αποτελέσματα πολύ κοντά στις θεωρητικές προβλέψεις.

Σχετική δημοσίευση :

- **"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)

B) Δισυσταδικά πολυμερικά μείγματα

Στην ομογενή περιοχή (περιοχή ανάμειξης), εξετάστηκε η σχέση ειδικών θερμοδυναμικών χαρακτηριστικών των συστατικών πολυμερών (όπως η διαφορά στην χαρακτηριστική θερμοκρασία της υαλώδους μετάπτωσης) με την πειραματικά παρατηρηθείσα *δυναμική ανομοιογένεια* σε τοπική κλίμακα, και παρουσιάστηκε ένα θεωρητικό μοντέλο για την περιγραφή αυτού του φαινομένου.

Σχετική δημοσίευση :

- **"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)

Στην περιοχή κοντά στον μακροφασικό διαχωρισμό μελετήθηκε ο μηχανισμός της πολλαπλής σκέδασης λόγω των ισχυρών διακυμάνσεων στην σύσταση σε διαφορετικά πολυμερικά μείγματα., σε συνάρτηση τόσο των ειδικών χαρακτηριστικών των συστατικών (όπως το μοριακό βάρος και η ενυπάρχουσα οπτική ανισοτροπία), όσο και της ιδιαίτερης

θερμοδυναμικής κατάστασης (απόσταση από το κρίσιμο σημείο διαχωρισμού) του κάθε μείγματος. Επιχειρήθηκε η θεωρητική (αναλυτική και αριθμητική) περιγραφή του φαινομένου, τα αποτελέσματα της οποίας συγκρίθηκαν με επιτυχία με το πείραμα.

Σχετική δημοσίευση :

- **"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)

Στην κατάσταση των δύο φάσεων, παρουσιάστηκε μια συστηματική μελέτη σε τήγματα δισυσταδικών πολυμερικών μειγμάτων, τόσο τύπου UCST (Upper Critical Solution Temperature), όσο και τύπου LCST (Lower Critical Solution Temperature) και περιγράφηκε πώς, μέσω της μελέτης της δυναμικής σε τοπική κλίμακα είναι δυνατόν, να γίνει μια λεπτομερής περιγραφή των χαρακτηριστικών των δύο φάσεων, δίνοντας πληροφορία, για την θερμοδυναμική κατάσταση του μείγματος και για την εξάρτηση της σχετιζόμενης μορφολογίας από τα ειδικά χαρακτηριστικά του μείγματος και των συστατικών του.

Σχετική δημοσίευση :

- **"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)

Γ) Αστεροειδή πολυμερή

Μελετήθηκε η στατική και δυναμική συμπεριφορά τμημάτων αστεροειδών πολυμερών με μεγάλο αριθμό βραχιόνων (arms), τόσο πειραματικά (σκέδαση ακτίνων X και ρεολογικές μετρήσεις) όσο και με Monte Carlo προσομοιώσεις. Δείχτηκε ότι τα συστήματα αυτά αυτοοργανώνονται σε μια μορφή "χαλαρής τάξης" (liquid-like ordering) επιδεικνύοντας χαρακτηριστικά απλών υγρών αλλά σε μακρομοριακή πλέον κλίμακα.

Σχετική δημοσίευση

- **"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)

Περιγραφή της ερευνητικής εργασίας σε μεταδιδακτορικό στάδιο

A) Συνεργασία με I.T.E. - ΙΗΔΛ

Σύνθετα υλικά

Στον τομέα των συνθέτων υλικών μελετήθηκαν οι επιπτώσεις στην τοπικής κλίμακας δυναμική συμπεριφορά, πολυμερικών αλυσίδων σε συνθήκες περιορισμένης γεωμετρίας. Οι διαστάσεις περιορισμού ήταν της τάξης των 1.5 έως 2 nm. Βρέθηκε ότι ο νανοσκοπικός περιορισμός επέφερε σημαντικές αλλαγές στην δυναμική συμπεριφορά. Συγκεκριμένα ανιχνεύτηκε ένας νέος τρόπος δυναμικής χαλάρωσης, χαρακτηριστικής χρονικής κλίμακας πολύ μικρότερης, και εξάρτησης από την θερμοκρασία πολύ διαφορετικής από την αντίστοιχη της τοπικής κίνησης του μη περιορισμένου υλικού, προσφέροντας έτσι νέες

προοπτικές για την κατανόηση θερμοδυναμικών και μικρορεολογικών ιδιοτήτων τεχνολογικά σημαντικών συστημάτων που βρίσκονται υπό παρόμοιες συνθήκες (όπως στην περίπτωση πολυμερικών υλικών σε λεπτά υμένια –films-)

Σχετικές δημοσιεύσεις

- **"Nanoscopic confinement effects on local dynamics"**
S. H. Anastasiadis, K. Karatasos, G. Vlachos, E. Manias, E. P. Giannelis
Phys. Rev. Lett., **84**(5), 915 (2000)
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"Confinement Effects on the Local Motion in Nanocomposites"
S. H. Anastasiadis, K. Karatasos, G. Vlachos, E. Manias, and E. P. Giannelis
In *"Dynamics in Small Confining Systems IV"*, J. M. Drake, G. S. Grest, J. Klafter, and R. Kopelman, Eds.,
Materials Research Society Symposium Proceedings
Vol. **543**, 125-130, Pittsburgh, PA, (1999).
- S. H. Anastasiadis, K. Karatasos, G. Vlachos, E. Manias, and E. P. Giannelis
"Local Dynamics under Severe Confinement in Nanocomposites"
Polym. Mater. Sci. Eng., Amer. Chem. Soc. **82**, 211 (2000)

B) Πανεπιστήμιο Leeds, Dept. of Physics and Astronomy, and IRC in Polymer Science and Technology, Leeds, UK (Νοέμβριος 1997 – Μάρτιος 2000)

Το γενικότερο πλαίσιο της εργασίας που πραγματοποιήθηκε στο Πανεπιστήμιο του Leeds και το IRC ήταν η λεπτομερής μελέτη στατικών και δυναμικών ιδιοτήτων πολυμερικών συστημάτων χρησιμοποιώντας προσομοιώσεις με την τεχνική της Μοριακής Δυναμικής.

i) *Γραμμικά πολυμερικά συστήματα :*

Το πρώτο μέρος της ερευνητικής προσπάθειας επικεντρώθηκε στον σκοπό της βαθύτερης κατανόησης της στατικής και δυναμικής συμπεριφοράς στην τοπική κλίμακα του ενός μονομερούς και/η της μιας στατιστικής μονάδας σε γραμμικά πολυμερικά μοντέλα. Με την ανάπτυξη μιας νέας μεθόδου δημιουργίας αρχικών διαμορφώσεων πολυμερικών δειγμάτων, κατέστη δυνατή η παραγωγή χαλαρωμένων (τόσο στην τοπική όσο και στην κλίμακα ολόκληρης της αλυσίδας) τμημάτων πολυμερικών αλυσίδων διαφόρων μεγεθών, και σε διάφορες πυκνότητες. Εξετάστηκε η εξάρτηση της στατιστικής των μοριακών διαμορφώσεων από τα ιδιαίτερα μορφολογικά χαρακτηριστικά του μονομερούς αλλά και από την παραμετροποίηση της μεθόδου προσομοίωσης. Ερευνήθηκε με λεπτομέρεια η επίδραση ενδομοριακών (διαφορετικά μοριακά βάρη) και διαμοριακών (μεταβολή της πυκνότητας) παραγόντων στην δυναμική συμπεριφορά σε τοπική κλίμακα, ενώ έγινε για πρώτη φορά, μια ακριβέστερη περιγραφή των εμφανιζομένων διαδικασιών χαλάρωσης. Η ανάλυση αυτή είχε σαν αποτέλεσμα την καλύτερη κατανόηση της συνεισφοράς αργών μηχανισμών κίνησης στον επαναπροσανατολισμό (reorientation) μερών της αλυσίδας, χαρακτηριστικού μήκους της τάξης της μιας στατιστικής μονάδας, βοηθώντας στην ερμηνεία προσφάτων πειραμάτων Πυρηνικού Μαγνητικού Συντονισμού (NMR) σε παρόμοια συστήματα. Επιπλέον εξετάστηκε η επίδραση μιας άλλης θερμοδυναμικής παραμέτρου, αυτή της πίεσης, στην στατιστική των μοριακών διαμορφώσεων και στην δυναμική συμπεριφορά γραμμικών πολυμερικών μοντέλων.

Σχετικές δημοσιεύσεις

- **"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) (corresponding author)
- **"Slow modes in local polymer dynamics"**
K. Karatasos and D. B. Adolf
J. Chem. Phys. **112**(19), 8225,(2000) (Communication) (corresponding author)
- **"An Investigation into the local segmental dynamics of Polyethylene: an isothermal/isobaric Molecular Dynamics "**
 S. Hotston, D. B. Adolf, K. Karatasos
J. Chem. Phys. **115**(5), 2359, (2001)

ii) Πολυμερικά μοντέλα της τοπολογίας των δενδριμερών

Στο δεύτερο μέρος εξετάστηκε η επίδραση μιας διαφορετικής τοπολογίας , αυτής των δενδριμερών, στην δυναμική τόσο σε τοπική κλίμακα, όσο και στην κλίμακα ολόκληρου του μορίου, καθώς και η συσχέτιση των δυναμικών ιδιοτήτων με τις φυσικές ιδιότητες των υλικών αυτών. Δόθηκε έμφαση στην μελέτη της επίδρασης του μεγέθους (μοριακού βάρους) και της τοπολογίας, στους μηχανισμούς που καθορίζουν την δυναμική και τις ιδιότητες μεταφοράς και διάχυσης σε διαλύματα. Η αναγνώριση και η περιγραφή των μηχανισμών αυτών αναμένεται να οδηγήσει στην εκμετάλλευση τέτοιων υλικών ως οχήματα για μεταφορά και επιλεκτική αποδέσμευση φαρμακευτικών ουσιών σε βιολογικές εφαρμογές, αλλά και σε μια μεγάλη γκάμα εφαρμογών ως συμβατοποιητές άλλων πολυμερικών συστημάτων και ως εξειδικευμένων λιπαντικών με ελεγχόμενη δράση.

Σχετική δημοσίευση

- **"Statics and Dynamics of model dendrimers as studied by molecular dynamics simulations"**
K. Karatasos, D. B. Adolf and G. R. Davies
J. Chem. Phys. (2001) **115**, 5310, (2001) (corresponding author)

Γ) Πανεπιστήμιο Βρυξελλών, Τμήμα Φυσικής Πολυμερών (Μάρτιος 2000-Ιούνιος 2001)

Στα πλαίσια του ευρωπαϊκού προγράμματος

«New Routes to Understanding Polymer Materials using Experiments and Realistic Modelling» η ερευνητική προσπάθεια στο Πανεπιστήμιο των Βρυξελλών επικεντρώνεται στην βαθιά κατανόηση των φυσικών ιδιοτήτων τεχνολογικά σημαντικών πολυμερών, όπως Πολυεθυλένιο (PE), Πολυισοβουτυλένιο (PIB), Πολυπροπυλένιο (PP), και Πολυβινυλοχλωρίδιο (PVC), χρησιμοποιώντας ρεαλιστικές (διατηρώντας όλη την ατομική λεπτομέρεια) τεχνικές μοριακών προσομοιώσεων. Στα πλαίσια αυτής της προσπάθειας, έγινε λεπτομερής μελέτη του PIB τα αποτελέσματα της οποίας συγκρίθηκαν με πειράματα από μετρήσεις Πυρηνικού Μαγνητικού Συντονισμού (NMR) σκέδασης νετρονίων και Διηλεκτρικής Φασματοσκοπίας. Με την δυνατότητα της επακριβούς μελέτης που προσφέρουν αυτού του είδους οι προσομοιώσεις, και με την ανάπτυξη νέων μεθόδων ανάλυσης της στατικής και δυναμικής συμπεριφοράς, ερευνήθηκαν τα χαρακτηριστικά των μηχανισμών που σχετίζονται με το φαινόμενο της υαλώδους μετάπτωσης, και κατέστη δυνατό να αναγνωριστούν οι βασικές αιτίες για τις ξεχωριστές ιδιότητες του πολυμερούς αυτού (πχ η πολύ χαμηλή θερμοκρασία υαλώδους μετάπτωσης). Επίσης έγινε δυνατή η ερμηνεία φαινομενικά αντικρουομένων παρατηρήσεων από διαφορετικές πειραματικές τεχνικές τόσο όσον αφορά στην κλίμακα του μονομερούς, όσο και στην κίνηση της ομάδας του μεθυλίου,

Karatasos K.

οδηγώντας σε μια γενικευμένη περιγραφή της δυναμικής του συμπεριφοράς. Η ερευνητική προσπάθεια συνεχίστηκε προχωρώντας συστηματικά σε μια απευθείας σύγκριση μεταξύ πειράματος και προσομοίωσης όσον αφορά τους μηχανισμούς που περιγράφουν το PP, το PE και το PVC, με σκοπό να αναγνωριστεί ο ρόλος των ατομικών διαφορών στην εκδήλωση των ιξωδοελαστικών ιδιοτήτων των πολυμερών αυτών. Μια τέτοια λεπτομερής κατανόηση των μηχανισμών που ευθύνονται για την εμφάνιση των ιδιοτήτων αυτών των υλικών, εντάσσεται στο γενικότερο πλαίσιο για την δυνατότητα εξαρχής συνθέσεως υλικών με επιθυμούμενες ιδιότητες.

Σχετικές δημοσιεύσεις

- **"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)
- **"Polyisobutylene dynamics revisited"**
K. Karatasos, and J.-P. Ryckaert
Macromolecules **34**, 7232 (2001) (Communication) (corresponding author)
- **"Methyl dynamics and β -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)
- **"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)

Φεβρουάριος 2003 – Απρίλιος 2008 (Λέκτορας στο τμ. Χημικών Μηχανικών του Α.Π.Θ.)

Στην εργασία

"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)

γίνεται μια συνδυασμένη προσπάθεια περιγραφής της τοπικής δυναμικής του πολυεθυλενίου με χρήση μοριακών προσομοιώσεων και σκέδασης νετρονίων. Εξετάζονται τα όρια εφαρμογή παραδοσιακών μεθόδων ανάλυσης των φασμάτων στο χώρο των συχνοτήτων και τα αποτελέσματα συγκρίνονται με την λεπτομερέστερη ανάλυση των αναλόγων δεδομένων από την μοριακή δυναμική. Στα πλαίσια αυτής της σύγκρισης, δείχνεται ότι η πειραματικά παρατηρούμενη συμπεριφορά, μπορεί να περιγραφεί με περισσότερη λεπτομέρεια αν θεωρηθεί η ύπαρξη δύο χαρακτηριστικών διαδικασιών χαλάρωσης σε χαμηλά μεγέθη του διανύσματος σκέδασης οι οποίες συνδυάζονται σε μία γρήγορη διαδικασία στο όριο των μεγάλων μεγεθών του διανύσματος σκέδασης (μικρές χωρικές κλίμακες).

Στην εργασία

"Static and dynamic behavior in model dendrimer melts: toward the glass transition"

K. Karatasos

Macromolecules **38**, 4472-4483 (2005)

Karatasos K.

πραγματοποιείται μια εκτεταμένη και λεπτομερής μελέτη τηγμάτων υπερδιακλαδισμένων πολυμερών της δενδριμερούς τοπολογίας με σκοπό την κατανόηση της στατικής και δυναμικής συμπεριφοράς τους σαν συνάρτηση του μοριακού μεγέθους και της θερμοκρασίας. Παρατηρείται η ύπαρξη μιας μετάβασης που φέρει τα χαρακτηριστικά της υαλώδους μετάπτωσης πολυμερικών συστημάτων. Εξετάζονται οι επιδράσεις της μετάβασης αυτής στις στατικές και δυναμικές ιδιότητες των δενδριμερών και γίνεται προσπάθεια κατανόησης των μηχανισμών στους οποίους οφείλεται αυτή η συμπεριφορά.

Στην εργασία

"Glass Transition in Dendrimers"

K. Karatasos

Macromolecules **39**,4619-4626 (2006)

επιχειρείται μια λεπτομερής περιγραφή των μηχανισμών που υπεισέρχονται στην εκδήλωση του φαινομένου της υαλώδους μετάβασης στα δενδριμερή στην κατάσταση τήγματος με προσομοιώσεις μοριακής δυναμικής. Εξετάζεται ο ρόλος της ειδικής τοπολογίας των μορίων αυτών, στην ανάπτυξη μορφολογικών αλλά και δυναμικών ετερογενειών κατά την προσέγγιση στην υαλώδη μετάβαση, ενώ μελετάται και η επίδραση του μοριακού βάρους. Τα αποτελέσματα της μελέτης είναι σε συμφωνία με πρόσφατες πειραματικές εργασίες στα υλικά αυτά, ενώ και οι μηχανισμοί που περιγράφονται φαίνεται να εξηγούν την παρατηρούμενη συμπεριφορά.

Στην εργασία

"Segmental Dynamics under severe Connectivity Constraints: the Dendrimer Case"

K. Karatasos, A.V. Lyulin

Journal of Chemical Physics **125**, 184907 (2006)

Εξετάζεται ο ειδικός ρόλος του τοπολογικού περιορισμού που επιβάλλεται από την δενδριτική δομή στην τοπικής κλίμακας κίνηση. Τα παρατηρούμενα χαρακτηριστικά συγκρίνονται με την συμπεριφορά που παρατηρείται σε γραμμικά πολυμερή αλλά και σε άλλα μοριακά συστήματα που παρουσιάζουν το φαινόμενο της υαλώδους μετάβασης (glass transition), ενώ επιχειρείται και ο προσδιορισμός του ρόλου διαφορετικών παραγόντων (μέγεθος μορίου, τοπολογία, θερμοδυναμική κατάσταση) στους μηχανισμούς πραγμάτωσης της κίνησης σε αυτήν την κλίμακα.

Στην εργασία

"Computational polymer dynamics via DL_POLY" (άρθρο ανασκόπησης μετά από πρόσκληση του εκδότη)

Adolf DB, Butler SN, Drew PM, Hotston S, Karatasos K

MOLECULAR SIMULATION **32** (12-13): 1017-1023, (2006)

Παρουσιάζεται μια ανασκόπηση των εργασιών σε Μοριακή Δυναμική με τη χρήση του προγράμματος ανοικτού κώδικα DL_POLY στο πεδίο της φυσικής πολυμερών. Σχολιάζονται συμπεράσματα που αφορούν τη στατική και τη δυναμική συμπεριφορά από προσομοιώσεις γραμμικών και πολυδιακλαδισμένων πολυμερικών συστημάτων, καθώς και από έρευνες για την διάχυση μικρών μορίων μέσα σε πολυμερικές μήτρες

Στην εργασία

"Non-Gaussian nature of Glassy Dynamics by Cage-to-Cage Motion"

Karatasos K.

B. Vorselaars, A.V. Lyulin, K. Karatasos and M. A. J. Michels

Physical Review E **75**, 011504 (2007)

Παρουσιάζεται ένα θεωρητικό μοντέλο με σκοπό την κατανόηση του μη-Gaussian χαρακτήρα της κίνησης κοντά στην περιοχή της υαλώδους μετάπτωσης για διαφορετικές κατηγορίες υλικών. Τα βασικά συμπεράσματα του μοντέλου φαίνεται να είναι συμβατά με την συμπεριφορά που παρατηρείται σε συστήματα πολύ διαφορετικής τοπολογίας όπως κολλοειδή, πολυμερή, δενδριμερή υποδεικνύοντας κάποιο κοινό πλαίσιο συμπεριφοράς κοντά στην υαλώδη μετάβαση.

Στην εργασία

“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)

Διεξάγεται μια συστηματική έρευνα των επιπτώσεων της μοριακής τοπολογίας καθώς και του μεγέθους, σε στατικές και δυναμικές ιδιότητες συμπλεγμάτων φορτισμένων υπερδιακλαδισμένων πολυμερών με αντίθετα φορτισμένες γραμμικές αλυσίδες, με την μέθοδο της Brownian δυναμικής. Διαπιστώνεται ότι με την χρήση μορίων διαφορετικής αρχιτεκτονικής, είναι δυνατόν να ελεγχθούν ιδιότητες όπως το μέσο μέγεθος, η ανισοτροπία του σχήματος καθώς και οι χαρακτηριστικοί χρόνοι χαλάρωσης σε τοπική και σε εκταταμένη κλίμακα. Οι ιδιότητες αυτές είναι κρίσιμες όσον αφορά τη χρήση πολυηλεκτρολυτικών συμπλεγμάτων σε μια πληθώρα τεχνολογικών και βιοϊατρικών εφαρμογών.

Στην εργασία

“Self Organisation in Dendrimer Polyelectrolytes”

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

εξετάζεται με τη χρήση προσομοιώσεων μοριακής δυναμικής η συμπεριφορά αραιών πολυηλεκτρολυτικών διαλυμάτων δενδριμερών 3^{ns} και 4^{ns} γενεάς (με ύπαρξη διαλύτη και αντισταθμιστικών ιόντων), υπό συνθήκες μεταβαλλόμενης ισχύος των ηλεκτροστατικών αλληλεπιδράσεων. Παρατηρείται πέρα από ένα χαρακτηριστικό κατώφλι της ισχύος των αλληλεπιδράσεων Coulomb, τα δενδριμερή αυτοοργανώνονται σε κυβικές φάσεις της FCC και BCC μορφής. Επιπρόσθετα, μελετάται η διαδικασία συμπύκνωσης των αντισταθμιστικών ιόντων γύρω από τα δενδριμερή και διαπιστώνεται ότι η αυτοοργάνωση των δενδριμερών, επέρχεται σαν αποτέλεσμα του συνδυασμού χωρικών συσχετίσεων των ιόντων γύρω από αυτά, αλλά και της «απελευθέρωσης» σωματίων διαλύτη από το εσωτερικό της δενδριτικής δομής. Οι διεργασίες αυτές επηρεάζουν το ενεργό φορτίο των δενδριμερών, και δημιουργούν κατά μέσο όρο κατάλληλες ενεργές αλληλεπιδράσεις μεταξύ των δενδριμερών μορίων οι οποίες και οδηγούν στο φαινόμενο της αυτοοργάνωσής τους.

Μάιος 2008 - τώρα (Επ. Καθηγητής επί θητεία στο τμ. Χημικών Μηχανικών του Α.Π.Θ.)

Στην εργασία

“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)

μελετάται με την μέθοδο της Brownian δυναμικής, το φαινόμενο της «υπερφόρτισης» (overcharging) σε συμπλέγματα γραμμικών πολυηλεκτρολυτών με υπερδιακλαδισμένα πολυμερή. Εξετάζεται η επίδραση της τοπολογίας των υπερδιακλαδισμένων πολυμερών και του μήκους της γραμμικής αλυσίδας στο παραπάνω φαινόμενο, ενώ επιχειρείται και η θεωρητική περιγραφή των συστημάτων αυτών. Τα αποτελέσματα της παρούσας μελέτης, μπορεί να ληφθούν υπόψη σε εφαρμογές όπου τέτοια συστήματα πολυηλεκτρολυτικών συμπλεγμάτων παίζουν σημαντικό ρόλο, όπως για παράδειγμα στην μεταφορά και αποδέσμευση ουσιών βιολογικού ενδιαφέροντος στα κύτταρα.

Στην εργασία

“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)

Εξετάζεται η επίδραση της εφαρμογής διατμητικής τάσης σε συστήματα συμπλεγμάτων φορτισμένων υπερδιακλαδισμένων πολυμερών με γραμμικούς πολυηλεκτρολύτες. Τα μελετούμενα συστήματα φέρουν διαφορετικά μοριακά βάρη και τοπολογία ώστε να εξαχθούν επιπλέον συμπεράσματα για την επηρροή του μεγέθους και της γεωμετρίας στην απόκρισή τους σε διατμητική τάση. Η μελέτη γίνεται με την μέθοδο της προσομοίωσης με Brownian δυναμική. Η εφαρμογή διατμητικής τάσης καλύπτει ένα ευρύ πεδίο παραμορφώσεων, μέχρι το σημείο διαχωρισμού των συστατικών των συμπλεγμάτων, φανερώνοντας έτσι τα όρια μέσα στα οποία τα συμπλέγματα παραμένουν ανέπαφα υπό την επίδραση διάτμησης. Η εξέταση των δυναμικών τους ιδιοτήτων δείχνει την ύπαρξη μια σχέσης κλίμακας (scaling) στις δυναμικές ιδιότητες τόσο σε τοπική όσο και σε ολόκληρη την μοριακή κλίμακα. Η τοπολογία φαίνεται να παίζει σημαντικό ρόλο στον βαθμό απόκρισης των συστημάτων αυτών (παραμόρφωση σχήματος, δυναμική στην κλίμακα του μορίου) αποκαλύπτοντας έτσι τρόπους ελέγχου των μηχανικών τους ιδιοτήτων για την επίτευξη επιθυμούμενης συμπεριφοράς σε συνθήκες υδροδυναμικής παραμόρφωσης.

Στην εργασία

“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

Materials Science and Engineering: B **2008**, 152, 114

μελετάται η επίδραση της εφαρμογής μεταβαλλόμενης έντασης ηλεκτροστατικών αλληλεπιδράσεων στις στατικές ιδιότητες συμπλεγμάτων μεταξύ γραμμικών πολυηλεκτρολυτών και υπερδιακλαδισμένων πολυμερών διαφορετικών τοπολογιών με την μέθοδο της Brownian Δυναμικής. Από την παρούσα εργασία υποδυκνείεται ότι με κατάλληλη επιλογή της εσωτερικής δομής (τοπολογίας) του υπερδιακλαδισμένου πολυμερούς και με την εφαρμογή ενός εξωτερικού παράγοντα (εδώ της ισχύος των ηλεκτροστατικών αλλ/σεων) καθίσταται δυνατόν να ελεγχθούν ιδιότητες όπως τα γεωμετρικά χαρακτηριστικά, η κατανομή πυκνότητας και το μέγεθος των συμπλεγμάτων, ιδιότητες κρίσιμες για μια ευρεία γκάμα εφαρμογών στις οποίες μπορεί να χρησιμοποιηθούν τα εξεταζόμενα συστήματα.

Στην εργασία

“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

περιγράφεται η μελέτη θερμοδυναμικών χαρακτηριστικών ενός υπερδιακλαδισμένου πολυεστεραμιδίου με την μέθοδο της ανάστροφης αέριας χρωματογραφίας. Με την εφαρμογή της μεθόδου αυτής κατέστη δυνατόν να υπολογιστούν οι Flory-Huggins παράμετροι αλληλεπίδρασης καθώς και οι μερικές και ολικές παράμετροι διαλυτότητας σαν συνάρτηση της θερμοκρασίας. Η εφαρμογή αυτής της μεθοδολογίας για πρώτη φορά σε τέτοιου είδους συστήματα, αποδείχτηκε κατάλληλη για να περιγράψει τις μερικές αλληλεπιδράσεις λόγω δεσμών υδρογόνου, δυνάμεων διασποράς και ηλεκτροστατικών δυνάμεων με σχετικά μεγάλη ακρίβεια.

Στην εργασία

“Dynamics of counterions in Dendrimer Polyelectrolyte Solutions”

K. Karatasos and M. Krystallis

Journal of Chemical Physics **2009**, *130*, 114903

μελετάται διεξοδικά με την χρήση μοριακών προσομοιώσεων η δυναμική συμπεριφορά των αντισταθμιστικών ιόντων σε διαλύματα δενδριτικών πολυηλεκτρολυτών, σε συστήματα με διαφορετική ισχύ των ηλεκτροστατικών αλληλεπιδράσεων. Περιγράφονται οι δυναμικές διαδικασίες που υπεισέρχονται στον σχηματισμό αλλά και στην συμπεριφορά της ιοντικής ατμόσφαιρας γύρω από τα φορτισμένα δενδριμερή, τόσο στην αυτόνομη όσο και στην συνεργαστική κίνηση των ιόντων. Δείχνεται για πρώτη φορά μια σχέση κλίμακας που συνδέει τον συντελεστή διάχυσης των ιόντων αλλά και των δενδριμερών με την ένταση των ηλεκτροστατικών αλληλεπιδράσεων αλλά και ο συσχετισμός των διαφορετικών χρονικών κλιμάκων στην δυναμική των ιόντων. Γίνεται ποιοτική σύγκριση με πειραματικά αποτελέσματα σε συστήματα φορτισμένων κολλοειδών αλλά και άλλων πολυμερικών πολυηλεκτρολυτικών συστημάτων και διαπιστώνεται καλό επίπεδο συμφωνίας.

Στην εργασία

“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

παρουσιάζεται για πρώτη φορά μια λεπτομερής εξέταση ενός υπερδιακλαδισμένου πολύ(εστεραμιδίου) σε κατάσταση τήγματος μέσω πλήρως ατομικού μοριακού μοντέλου. Μελετώνται στατικές, δυναμικές και θερμοδυναμικές ιδιότητες και συγκρίνονται με πειράματα διαφορικής θερμιδομετρίας σάρωσης, ανάστροφης αέριας χρωματογραφίας και ρεολογίας, όπου διαπιστώνεται πολύ καλή συμφωνία. Με βάση την πολύ καλή συμπεριφορά του μοριακού μοντέλου στις παραπάνω ιδιότητες, η μελέτη επεκτείνεται στον χαρακτηρισμό του πολυμερούς ως προς τον σχηματισμό διαφορετικού είδους δεσμών υδρογόνου. Λαμβάνοντας υπόψη όλα τα αποτελέσματα της στατικής και δυναμικής συμπεριφοράς, καθίσταται δυνατή η ταυτοποίηση των μηχανισμών σε τοπική κλίμακα που είναι υπεύθυνοι για την εκδήλωση της μακροσκοπικής συμπεριφοράς του συστήματος και τίθεται η βάση για τον σχεδιασμό σε μοριακό επίπεδο παρόμοιων συστημάτων με επιθυμητές ιδιότητες.

Karatasos K.

Στην εργασία

“Electrostatically-driven Ordering in Model Dendrimer Polyelectrolytes: Effects of Concentration”

K. Karatasos and M. Krystallis

Macromol. Symp. , **2009**, 278, 32–39

εξετάζεται με την μέθοδο της μοριακής προσομοίωσης η επίδραση της αλλαγής της συγκέντρωσης των φορτισμένων δενδριμερών στην συμμετρία της δομής που προκύπτει από την αυτοοργάνωση των δενδριμερών με την επίδραση ηλεκτροστατικών αλληλεπιδράσεων. Μελετάται ο ρόλος της οργάνωσης των αντισταθμιστικών ιόντων γύρω από τα δενδριμερή, αλλά και η κινητική συμπεριφορά των δενδριμερών (διάχυση) σαν συνάρτηση της συγκέντρωσης και της ισχύος των ηλεκτροστατικών αλληλεπιδράσεων. Διαπιστώνεται καλή συμφωνία με θεωρητικές προβλέψεις σε παρόμοια συστήματα πολυμερικών ηλεκτρολυτών ενώ συζητείται και ο ρόλος της κινητικής στον σχηματισμό της τελικής δομής.

Στην εργασία

“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. , 113, 10984–10993, **2009**

εξετάστηκαν οι μηχανισμοί που είναι υπεύθυνοι για την μη-ομοιοπολική πρόσδεση/εγκλεισμό ενός μη-στεροειδούς αντιφλεγμονώδους φαρμάκου, με δενδριμερές πολυ(αμιδο-αμινικού) τύπου 3^{ης} και 4^{ης} γενεάς, με την βοήθεια πλήρως ατομιστικών μοριακών προσομοιώσεων. Διαπιστώθηκε ότι η αποτελεσματικότητα του σχηματισμού συμπλεγμάτων δενδριμερούς/φαρμάκου εξαρτάται δραστικά από το pH του διαλύματος, ενώ διαπιστώθηκε και η μεταβολή της φύσης του μηχανισμού πρόσδεσης από ηλεκτροστατική σε κυριαρχούμενη από δεσμούς υδρογόνου. Επιπλέον, μελετήθηκε για 1^η φορά η δυναμική συμπεριφορά των μορίων του φαρμάκου και εκτιμήθηκαν οι χρονικές κλίμακες τόσο της κίνησης των ξεχωριστών μορίων, όσο και της συλλογικής κίνησης αυτών. Τα συμπεράσματα από την εργασία αυτή, βοηθούν στην ερμηνεία σχετικών πειραμάτων σε αυτά τα συστήματα, ενώ θέτουν και το γενικότερο πλαίσιο της αντίστοιχης συμπεριφοράς μιας μεγαλύτερης οικογένειας υδρόφοβων και ασθενώς όξινων φαρμακευτικών ουσιών.

Στην εργασία

“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**

Μελετώνται για πρώτη φορά με την μέθοδο της ανάστροφης αέριας χρωματογραφίας μια σειρά από αλειφατικού υπερδιακλαδισμένου πολυεστέρες (Boltorn® H20, H30 and H40) κάνοντας χρήση 13 διαφορετικών διαλυτών ως μόρια ανιχνευτές. Δεδομένα του όγκου κατακράτησης αναλύθηκαν για τον θερμοδυναμικό χαρακατηρισμό των πολυμερικών αυτών υλικών, οδηγώντας στον υπολογισμό ποσοτήτων όπως ο παράγοντας αλληλεπίδρασης Flory-Huggins, ο κατά βάρος συντελεστής ενεργότητας, καθώς και ο συνολικός αλλά και οι

επιμέρους παράγοντες διαλυτότητας και η εξάρτησή τους από τη θερμοκρασία. Τα αποτελέσματα της εν λόγω μελέτης εκτός του ότι παρέχουν νεά πληροφορία για τα συγκεκριμένα συστήματα, εκτιμάται ότι δείχνουν και τις τάσεις που ενδέχεται να ακολουθούν και άλλα πολυμερή της δενδριτικής τοπολογίας που φέρουν ανάλογες ενεργές ομάδες αλληλεπίδρασης.

Στην εργασία

“Local Dynamics and Hydrogen Bonding in Hyperbranched Aliphatic Polyesters”

I. Tanis and K. Karatasos

Macromolecules, 42, 9581 , 2009

εξετάζονται για πρώτη φορά σε πλήρως ατομιστικό επίπεδο με την βοήθεια προσομοιώσεων μοριακής δυναμικής, οι μηχανισμοί που σχετίζονται με την σύζευξη της τοπικής δυναμικής με το σχηματιζόμενο δίκτυο υδρογονικών δεσμών, για αλκίφατικούς υπερδιακλαδισμένους πολυεστέρες 2 διαφορετικών γενεών. Αποκαλύπτεται και περιγράφεται με λεπτομέρεια ο μηχανισμός σύζευξης των τοπικών κινήσεων (σε επίπεδο δεσμού) με τους σχηματιζόμενους υδρογονικούς δεσμούς, σε σχέση με την τοπολογία των υπερδιακλαδισμένων μορίων. Οι μηχανισμοί που περιγράφονται από τα αποτελέσματα των προσομοιώσεων, παρέχουν ένα ικανοποιητικό πλαίσιο ερμηνείας σχετικών πειραμάτων διηλεκτρικής φασματοσκοπίας και φασματοσκοπίας υπερέυθρου, τόσο ως προς την φύση των σχηματιζόμενων υδρογονικών δεσμών, όσο και στην δυναμική κλίμακα που σχετίζεται με αυτούς και την σύζευξή της με τις κινήσεις των πολυμερών σε τοπική κλίμακα.

Στην εργασία

“Modeling of Hyperbranched Polyesters as Hosts for the Multifunctional Bioactive Agent Shikonin”

I. Tanis, K. Karatasos, A. N. Assimopoulou and V. P. Papageorgiou

Physical Chemistry Chemical Physics, 2011, 13, pp 10808

γίνεται για πρώτη φορά προσπάθεια μοντελοποίησης μιας οικογένειας υπερδιακλαδισμένων πολυεστέρων οι οποίοι είναι και διαθέσιμοι εμπορικά, ως παράγοντες δέσμευσης του βιοδραστικού μορίου της Σικονίνης, σε πλήρη ατομιστική αναπαράσταση με την μέθοδο της Μοριακής Δυναμικής. Σε αυτή την εργασία εξετάζονται λεπτομερώς οι μηχανισμοί και οι συνθήκες κάτω από τις οποίες ευνοείται η δημιουργία συμπλέγματος μεταξύ των πολυεστέρων και της Σικονίνης, ενώ διερευνούνται και οι επιδράσεις του μοριακού βάρους και των ιδιαίτερων τοπολογικών χαρακτηριστικών των πολυμερών καθώς και της συγκέντρωσης των πολυεστέρων στην διαδικασία της δέσμευσης.

Στην εργασία

“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

μελετάται η απόκριση των μορφολογικών και δυναμικών χαρακτηριστικών ενός συμμετρικού ως προς τη σύσταση μείγματος περιφερειακά φορτισμένων δενδριμερών 3^{ης} και 4^{ης} γενεάς σε αναπαράσταση ενωμένων ατόμων, στις αλλαγές της ισχύος των ηλεκτροστατικών

αλληλεπιδράσεων. Εξετάζεται υπό ποιες συνθήκες τα συστατικά του μείγματος αυτοοργανώνονται σε πλεγματικές δομές διαφορετικών χαρακτηριστικών, ενώ καθορίζεται και η αντίστοιχη δυναμική συμπεριφορά των συστατικών στην μοριακή κλίμακα. Με την παρούσα μελέτη δείχνεται πως, με τον έλεγχο της ισχύος των ηλεκτροστατικών αλληλεπιδράσεων, είναι δυνατόν να ελεγχθούν οι ιδιότητες αυτοοργάνωσης τέτοιων «χαλαρών» κολλοειδών συστημάτων

Στην εργασία

“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. Pricl

Macromolecular Bioscience, 12, pp 225, 2012

εξετάζονται με τη χρήση πλήρως ατομιστικών μοντέλων και σε συνθήκες που προσομοιάζουν ρεαλιστικά συστήματα, συμπλέγματα δενδριμερών μορίων της πολυ(αμιδοαμιδικής) οικογένειας με μικρού μήκους RNA διπλής έλικας, σε υδατικό περιβάλλον με διαφορετικές τιμές pH. Εξετάζεται η επίδραση της τοπολογίας των δενδριμερών μορίων, της γενεάς (μέγεθος) του δενδριμερούς, καθώς και της τιμής του pH στις δομικές αλλαγές που επέρχονται στα συστατικά του συμπλεγματος αλλά και στην αποτελεσματικότητα της πρόσδεσης μεταξύ των δύο μορίων. Εξάγονται συμπεράσματα για τη σχετική συνεισφορά εντροπικών και ενθαλπικών παραγόντων στην αποτελεσματικότητα της πρόσδεσης και επισημαίνονται εκείνοι οι παράγοντες που ευνοούν τον σχηματισμό περισσότερο ευσταθών συμπλεγμάτων. Τα αποτελέσματα συγκρίνονται ποιοτικά με σχετικά πειράματα σε παρόμοια συστήματα.

Στην εργασία

Chimeric advanced drug delivery nano systems (chi-aDDnSs) 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

ο κύριος σκοπός ήταν η μελέτη των συμπλεγμάτων του βιοενεργού μορίου shikonin με μια ειδική κατηγορία υπεδριακλαδισμένων αλιφατικών πολυεστέρων, και η εξέταση της δυνατότητας εγκλεισμού των σχηματιζομένων συμπλεγμάτων σε νέους «χιμαιρικούς» λιποσωμιακούς φορείς, με τελικό σκοπό την χρήση τους ως οχήματα μεταφοράς για θεραπευτικούς σκοπούς. Μιας και είναι η πρώτη φορά που μελετώνται αυτά τα υδριδικά συστήματα ως φορείς παράδοσης του shikonin, δόθηκε έμφαση στην αποτελεσματικότητα και την επαναληψιμότητα του πρωτοκόλου παραγωγής τους, στο βαθμό αποδοτικότητάς τους όσον αφορά το ποσοστό παγίδευσης των συμπλεγμάτων μέσα στην λιποσωμιακή κοιλότητα, στην σταθερότητά τους, αλλά και στην *in vitro* μελέτη του ρυθμού απελευθέρωσης της φαρμακευτικής ουσίας από αυτούς τους φορείς. Τα αποτελέσματα της παρούσας μελέτης δείχνουν ότι πρόκειται για πολλά υποσχόμενα συστήματα στην παγίδευση και ελεγχόμενη αποδέσμευση της πολλαπλά βιοδραστικής ουσίας shikonin

Στην εργασία

Conformational effects in non-stoichiometric complexes of two hyperbranched molecules with a linear polyelectrolyte

Karatasos K.

εξετάζονται χαρακτηριστικά των διαμορφώσεων των συστατικών πολυηλεκτρολυτικών συμπλεγμάτων αποτελούμενων από γραμμικές αλυσίδες διαφορετικών μηκών, με 2 υπερδιακλαδισμένα πολυμερή τα οποία κατά προτίμηση φέρουν μεγαλύτερο ποσοστό διακλαδώσεων στην περιφέρειά τους. Τα χαρακτηριστικά της φυσικής προσρόφησης των γραμμικών αλυσίδων συσχετίζονται με τις αντίστοιχες διαμορφώσεις των γραμμικών πολυμερών και μελετώνται σαν συνάρτησης του μήκους της αλυσίδας τους. Τα αποτελέσματα συγκρίνονται με αυτά προηγούμενων εργασιών που αναφέρονται σε αντίστοιχα στοιχειομετρικά κτυμπλέγματα, καθώς και με αυτά από στοιχειομετρικά και μη στοιχειομετρικά συμπλέγματα στα οποία συμμετέχουν υπερδιακλαδισμένα πολυμερή τέλειας δένδριτικής τοπολογίας. Επισημαίνεται ο πολύ σημαντικός ρόλος της τοπολογίας των υπερδιακλαδισμένων μορίων στις παρατηρούμενες διαφορές, παρέχοντας έτσι πληροφορία για τον καλύτερο έλεγχο των φυσικών ιδιοτήτων τέτοιων συστημάτων.