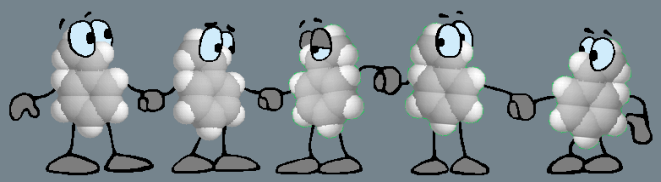
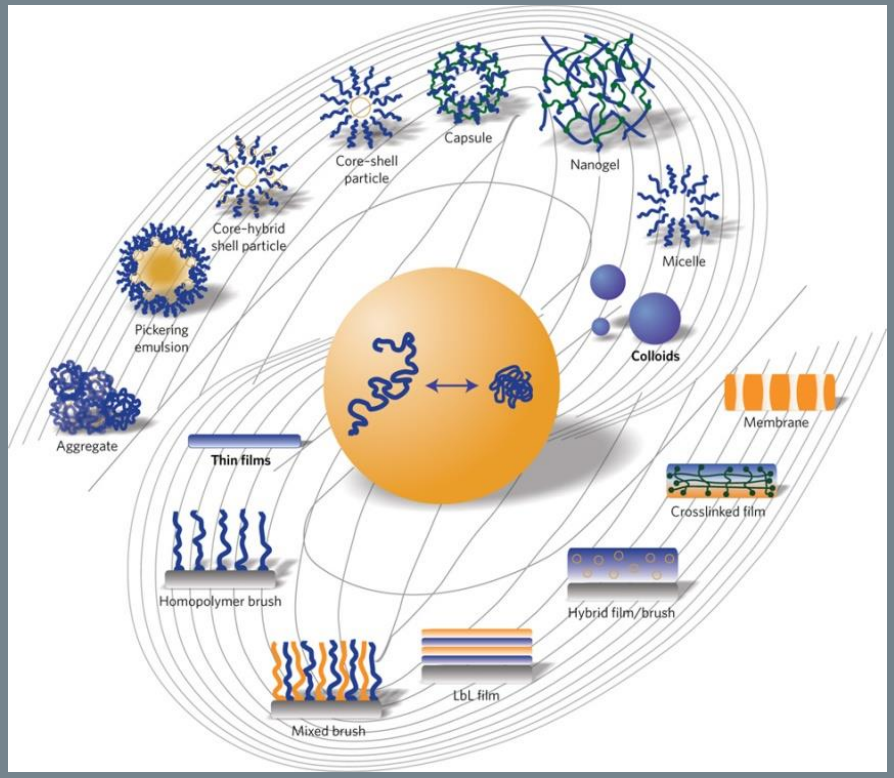
UNIVERSITY OF PATRAS
Department Of Chemical Engineering
ChemEngUP





Polymer Science and Technology

Vlasis Mavrantzas, George Staikos, Constantinos Tsitsilianis

General description of the Research Area

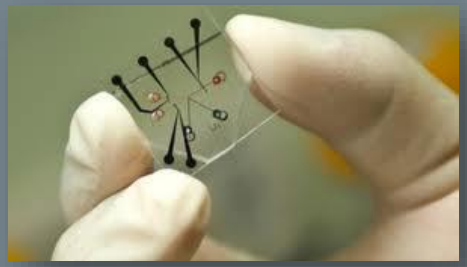
Polymer science is today a vibrant field. Its technological relevance is vast.

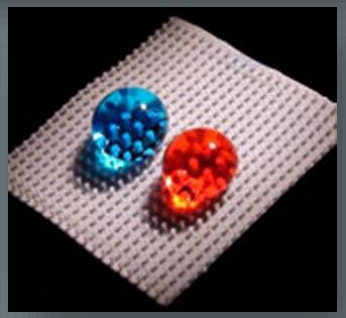
Polymeric materials exhibit a wealth of fascinating properties which are directly due to molecular behavior, i.e. the long chain nature of macromolecules.

Yet fundamental scientific questions and technological challenges abound, motivating extensive research activity word wide

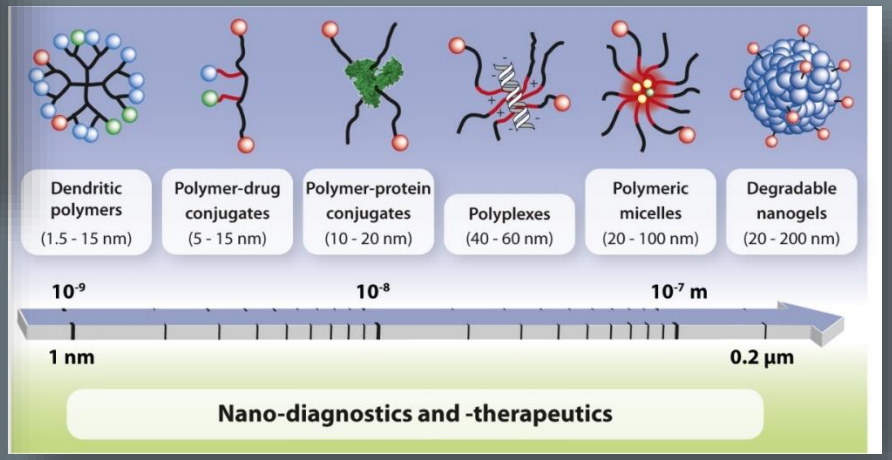
advanced materials

nanotechnology





biomedicine



Research Groups

- Lab of Statistical Thermodynamics and Macromolecules
  Prof. V. Mavrantzas

  Development and implementation of computational methods: Thermodynamic and rheological properties of polymers, Polymers at the interface.

- Organic Chemical Technology Lab
  Prof. G. Staikos

  Water-soluble polymers, Hydrogen-bonded interpolymer complexes, Colloidal nanoparticles.

- Polymer Lab
  Prof. C. Tsitsilianis

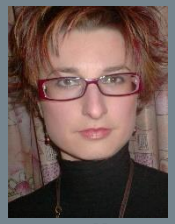
- Macromolecular engineering, responsive nanostructured self-assemblies: injectable hydrogels, micellar nanocariers.

Researchers

Post-Doc

Alexiadis Orestis

Post-Doc

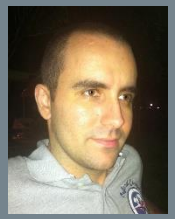


Karadima Katerina

Post-Doc

Tsalikis Dimitris

PhD student

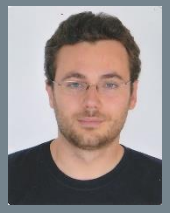


Anastassiou Alexandros

PhD student

Karahaliou Elena

PhD student

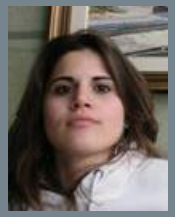


Koukoulas Thanasis

PhD student

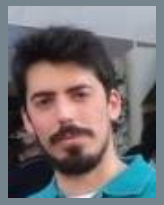
Skountzos Manolis

MSc student



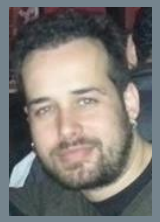
Tsourtou Flora

MSc student



Alatas Panayiotis

MSc student



Mermigkis Takis

5 post-Doc
7 PhD
3 MSc

PhD student

Theofanis Asimakopoulos

PhD student

Nicoleta-Oana Ciocoiu

PhD student

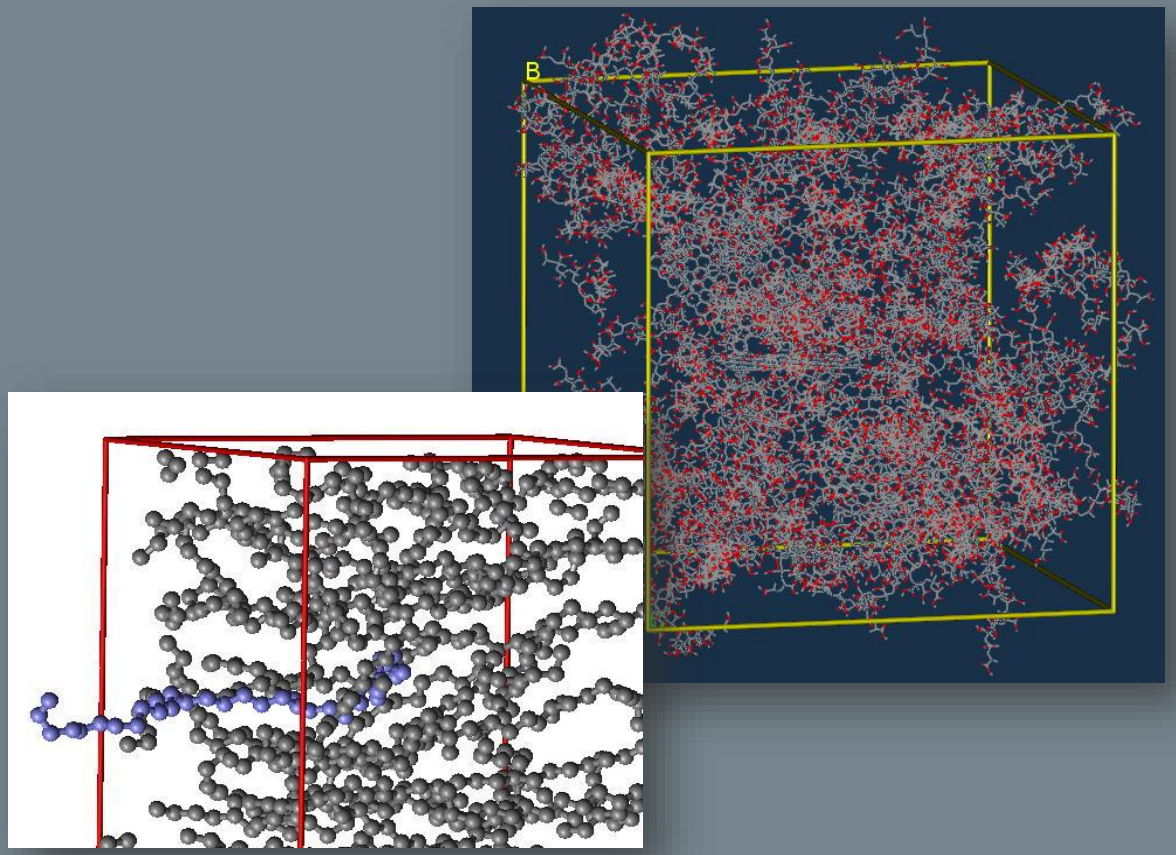
Sandra Gerboura

Post Doc

Teodora Popescu

Post Doc

Soledad Lencina



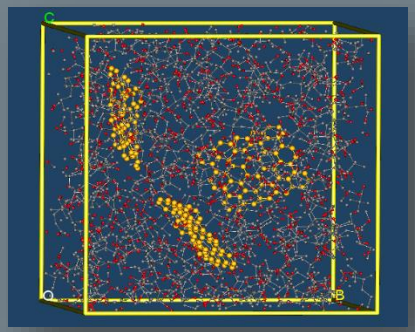
Research Group 1 Statistical Thermodynamics & Macromolecules

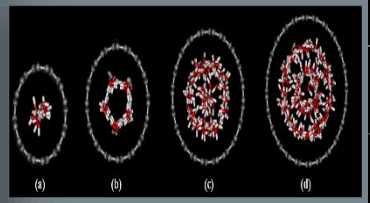
Atomistic Molecular Dynamics Simulations, Non-Equilibrium Thermodynamics

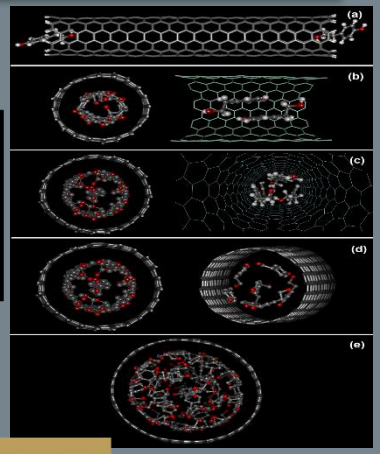
Research Activities LSTM group

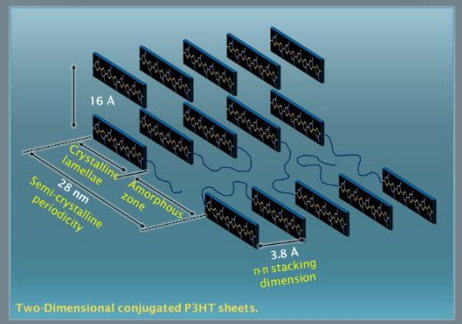
Simulation and Molecular-Constitutive Modeling of:

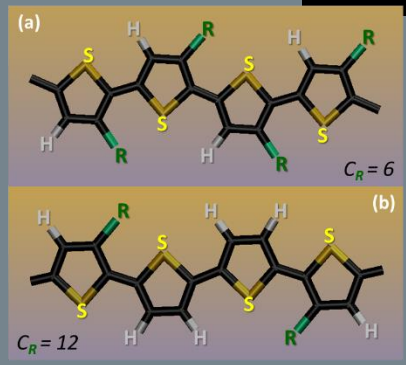
- ***Polymer/Graphene, Polymer/CNT nanocomposites***
- ***Polymer Semiconductors***
- ***Polymer Rings***
- ***High-MW Polymer Melt Viscoelasticity***
- ***Polymer Networks and Adhesion to substrates***

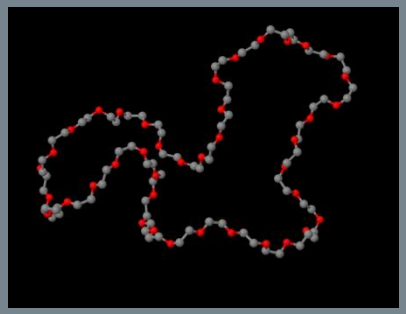


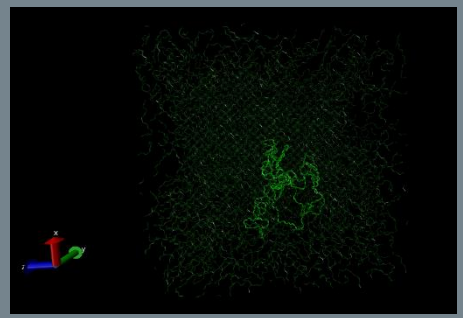












Molecular Dynamics of Regioregular P3HT

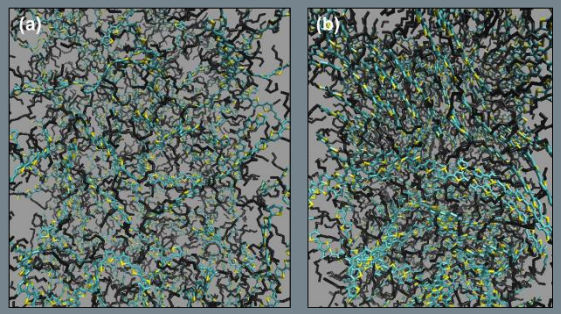
LSTM group

Motivation and scope: Unique opto-electrical properties, high carrier mobility ($0.1 cm^2/V\ s$) in the ordered state. OLED, OFET

Simulation predictions:

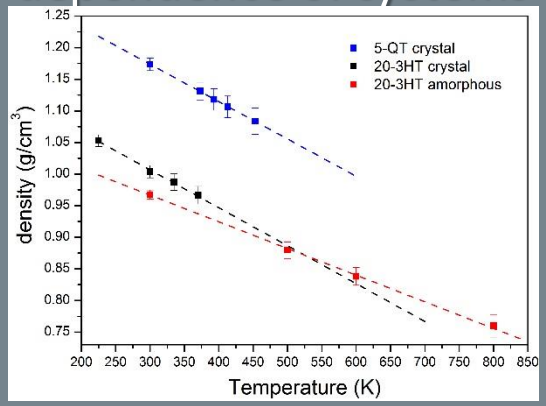
- Structure and morphological properties of Poly-alkyl-thiophenes (PATs)
- Periodicity and hierarchical ordering

Semi-crystalline transition in P3HT



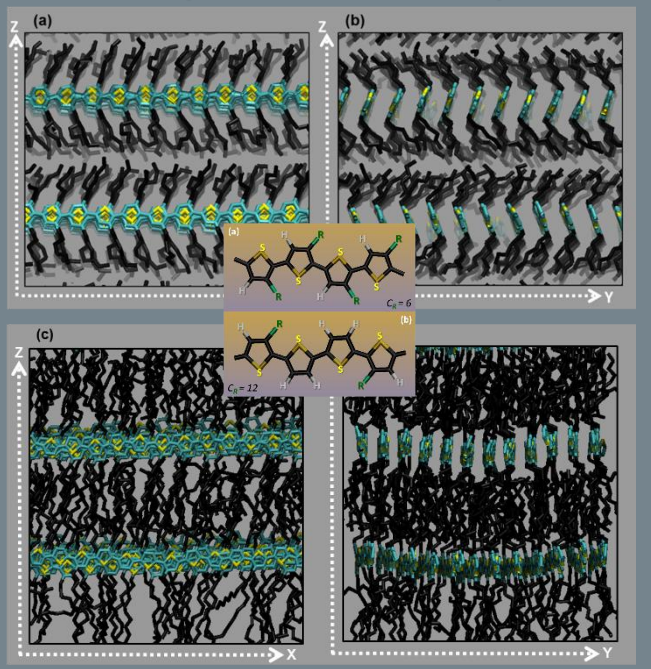
Typical snapshots of the (a and b) 3hexyl-20thiophene (20-3HT) system and (c and d) the 5-QT system at the end of a Molecular Dynamics simulation at 300K in the XZ projection and in the YZ projection respectively

Temperature dependence of systems

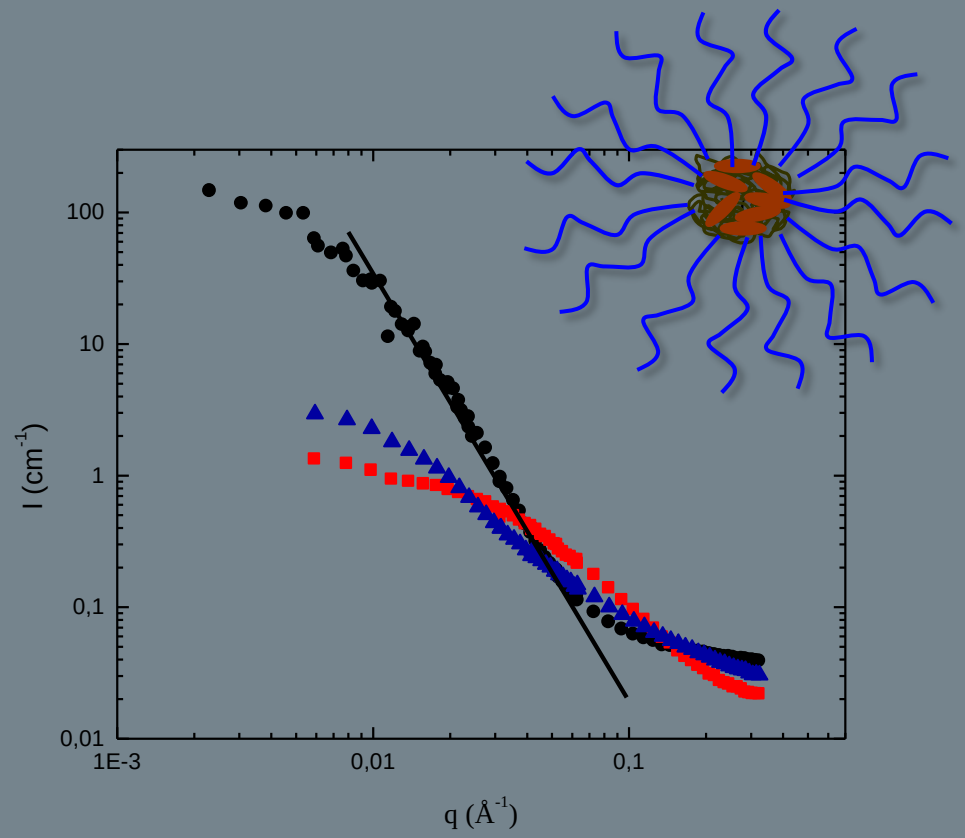


The density of 5-QT and 20-3HT crystal and 20-3HT melt as a function of simulation temperature

Side chain interdigitation (P3HT .vs. PQT)



Typical snapshots of the (a and b) 3hexyl-20thiophene (20-3HT) system and (c and d) the 5-QT system at the end of a Molecular Dynamics simulation at 300K in the XZ projection and in the YZ projection respectively

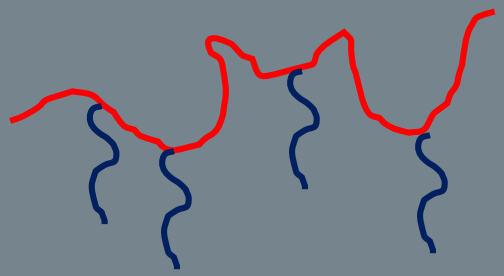


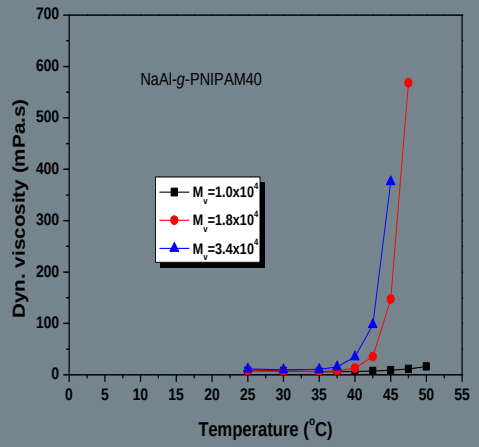
Research Group 2 Water-soluble polymers

Protein/polyelectrolyte complexes, Colloidal nanoparticles

Research Activities WsPol group

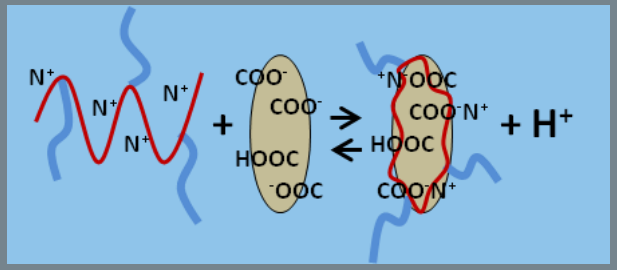
- Thermothickening systems

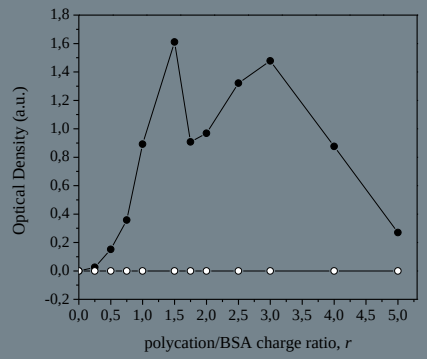


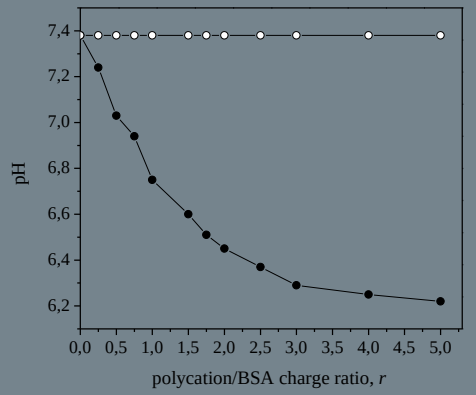


Sodium alginate-*graft*-PNIPAM Copolymers as thermothickening agents

- Bovine serum albumin/polycation complexe nanoparticles





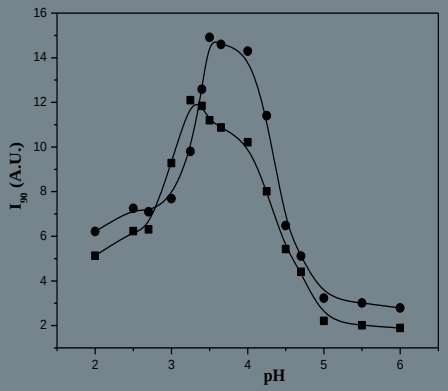


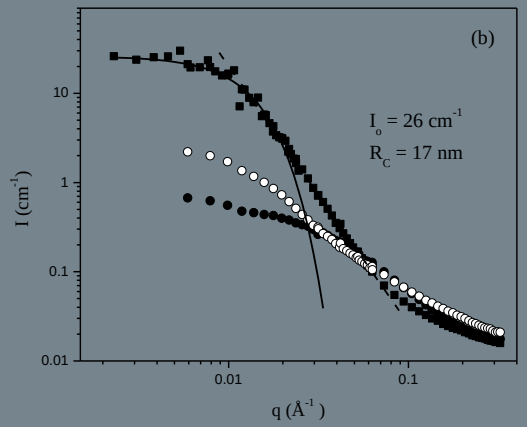
A complex formation study between bovine serum albumin and poly(methacrylamidopropyltrimethylammonium chloride)

Protein-polyelectrolyte complexes WsPol group

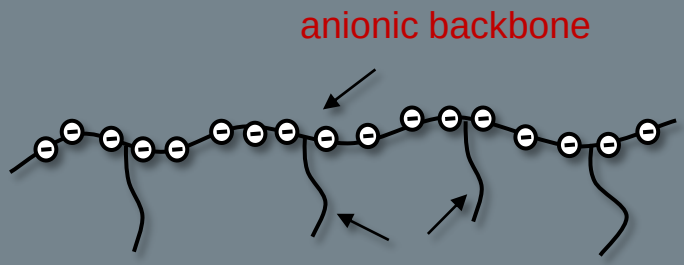
- Protein-polyelectrolyte colloidal nanoparticles

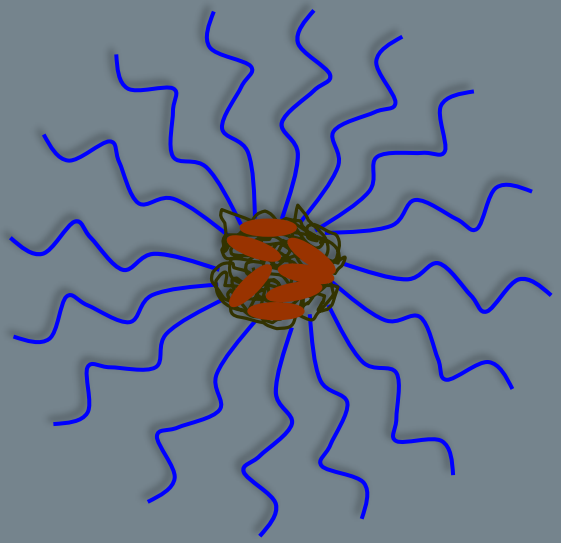
Polyelectrolytes, grafted with neutral hydrophilic chains interact with proteins forming soluble complexes. The resulted colloidal nanoparticles exhibit spherical core-shell structure

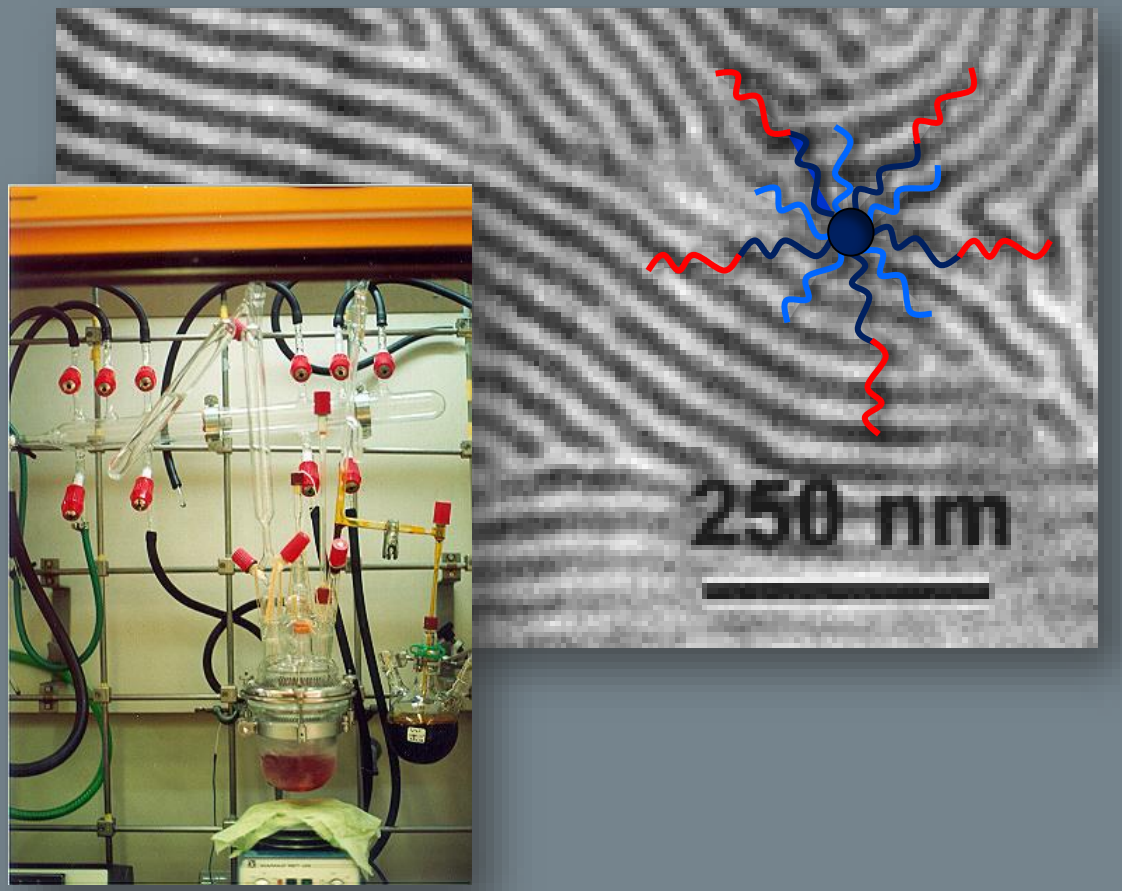




- Potential applications in Biomedicine: drug delivery





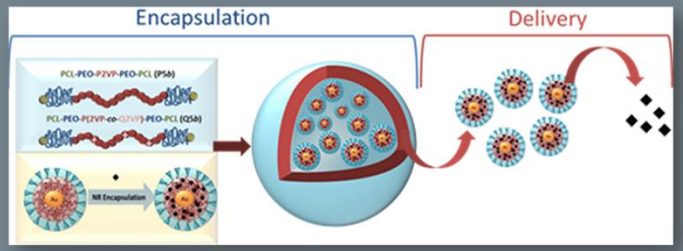


Research Group 3 Macromolecular Engineering

From tailor made polymers to tailor made nanostructured polymeric materials

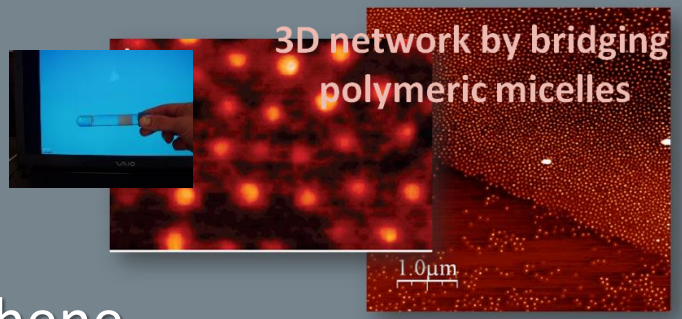
Research Activities MacroEng group

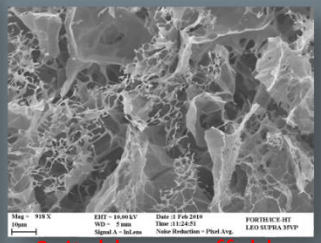
- Complex drug delivery systems



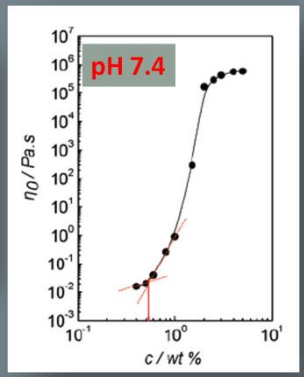
Controlled delivery of hydrophobic drug trough functionalized gold nanoparticles encapsulated in pH-sensitive polymersomes

- "smart" Injectable hydrogels

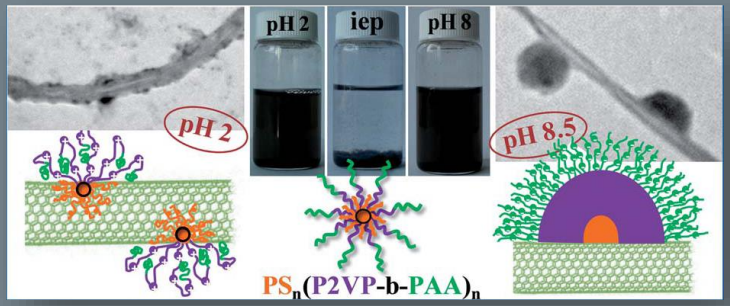


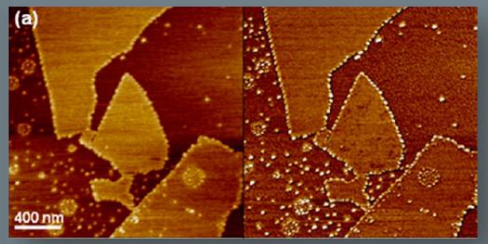


Suitable as scaffold for tissue engineering



- Polymer/CNT,Graphene nanohybrids

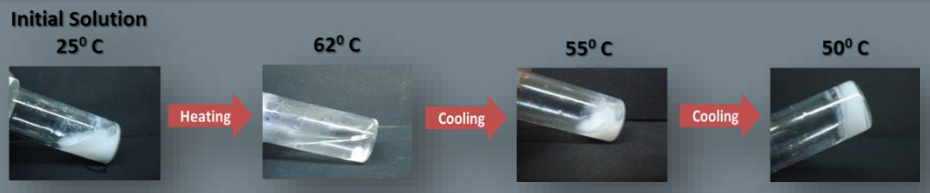




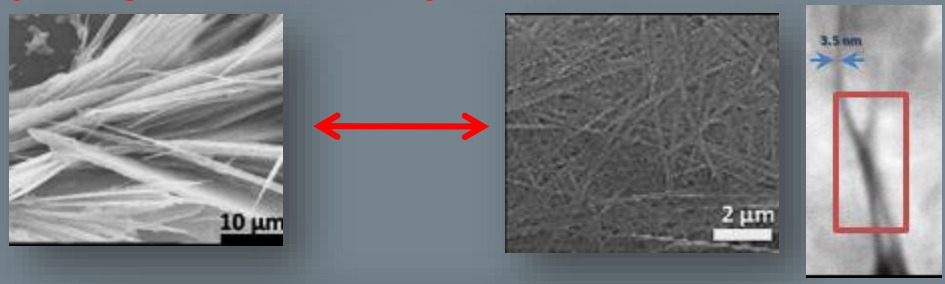
Polypeptide-based biodegredable hydrogels

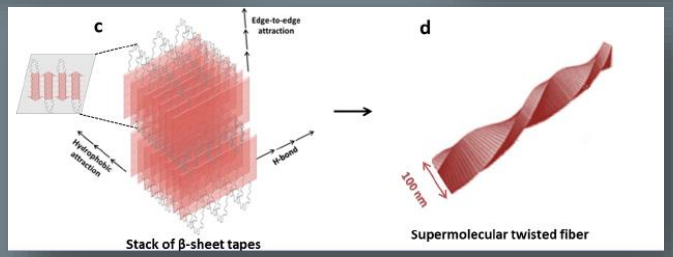
MacroEng group

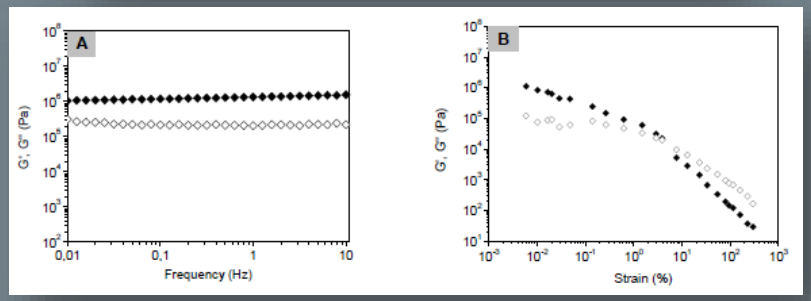
- **Motivation:** Biodegredable physically crosslinked hydrogel for biomedical applications.
- **Design:** Triblock copolymer composed of polypeptide sequences.
  PAla-PGA-PAla
- Hierarchical self-assembly of triblock copolypeptide , triggered by pH and salinity, leads to a 3D transient network of superfibers composed of β-sheets, Ala/random coil, GA secondary structures of the polypeptide chains.
- **Potential applications:** drug delivery, tissue engineering.



Physiological conditions: pH 7.4, T=37 ºC, 0.15M salt







Long-lasting collaborations

LSTM

- School of Chemical Engineering, National Technical University of Athens (Prof. Doros Thedoorou)
- University of Crete, Department of Materials Science (Prof. Dimitris Vlassopoulos)
- Department of Materials, ETH, Zürich, Switzerland (Prof. Hans Christian Öttinger, Prof. Martin Kröger)
- Norwegian University of Science and Technology (NTNU), Trondheim, Norway (Prof. Zhiliang Zhang)
- Department of Applied Physics, University of Tokyo, Japan (Prof. Masao Doi)
- Dow Chemical Company, Terneuzen, The Netherlands (Dr. Rudy Koopmans)
- University of Delaware, Department of Chemical Engineering, Newark, DE, USA (August 1999, with Prof. Antony Beris)
- ESPCIS, Paris, France (Prof. Costantino Creton)
- Lyondell Basel Industries (LBI), Frankfurt, Germany (Dr. Iakovos Vittorias)

WsPol

- Romanian Academy, Petru Poni Institute of Macromolecular Chemistry, Physical Chemistry Polymers Laboratory, Iasi, Romania
- Department of Polymer Science, University Politehnica, Bucharest, Romania
- Institute of Physical Chemistry, "I. G. Murgulescu" Romanian Academy, Bucharest, Romania
- Department of Macromolecular Compounds, Faculty of Applied Chemistry and Materials Science, University Politehnica, Bucharest, Romania

MacroEng

- Institute "Charles Sadron", Strasbourg, France.
- Dept. of Polymer Chemistry, University of Groningen, The Netherlands.
- Dept. of Physics & Macromolecular Chemistry, Charles University, Prague Czech Republic.
- Dept. of Physical Chemistry 1, Lund University, Sweden.
- Institut für Polymerforschung, Dresden, Germany.
- Τμήμα Χημείας, Πανεπιστήμιο Κύπρου.
- Dept. of Chemistry, Clarkson University, USA.
- Dept. of Materials Science and Engineering, Iowa State University, USA.
- School of Materials Science and Engineering, Georgia Institute of Technology, USA
- Université Européenne de Bretagne, LIMATB Equipe Rhéologie, Brest, France.
- Technische Universität München, Physikdepartment, Fachgebiet Physik weicher Materie, Garching, Germany.

Current Research Projects

- ΘΑΛΗΣ (ΕΣΠΑ): Graphene and its nanocomposites: production, properties and applications
  ΙΕΧΜΗ/ΙΤΕ, Τ.ΧΗΜ.ΜΗΧ/Π.Π., Τ.ΜΗΧ.ΑΕΡ.ΜΗΧ./Π.Π, Τ.ΗΛΕΚ/ΤΕΙ ΚΡ.
  Total budget: 600 k€
- ΑΡΙΣΤΕΙΑ (ΕΣΠΑ): Γενικευμένη Μέθοδος Προσομοίωσης της Αυτο-Οργάνωσης σε Νανοδομημένα Πολυμερικά Συστήματα-GENESIS
  Total budget: 300 k€
- ΣΥΝΕΡΓΑΣΙΑ (ΕΣΠΑ) **«Bioref»** Ανάπτυξη βιοδιυλιστηρίου για την αξιοποίηση υπολειμμάτων παραγωγής βιοντήζελ προς βιοαποικοδομήσιμα πολυμερή και προϊόντα υψηλής προστιθέμενης αξίας.
  ΑΡΓΩ ΑΕΒΕ, ΕΤΤΕΤ/ΓΠΑ, ΙΕΧΜΗ/ΙΤΕ, CHIMAR HELLAS AE, ΠΕΤΤΑΣ Π.Ν. ΑΒΕΕ
  Total budget: 626 k€
- EC (FP7-NMP-2009-SMALL-3): Development of the next generation membrane bioreactor system (BioNexGen)
  HSKA (Coordinator), CNR-ITM, UON, FORTH, SEZ, MN, IZTECH, ABU, CMRDI, CBSX LSTM
  budget: 60 kEuro

Current Research Projects

- ΗΡΑΚΛΕΙΤΟΣ ΙΙ (ΕΣΠΑ): Relations of structure, viscoelastic, mechanical, and adhesive properties of polyacrylics on solid substrates via molecular dynamics in atomistic detail
  Total budget: 45 k€
- MODIFY: Multi-scale modeling of interfacial phenomena in acrylic adhesives undergoing deformation
  U Patras, DOW, LBI, ETH-Z, UCL, CNRS, ESPCI, MIT, Utokyo,
  Total budget: 3.342 M€
- MMM@HPC:Multiscale material modelling on high performance computer architectures
  STFC, Umons, CEA, KIT, NOKIA, CSC, SONY, CINECA, Upatras
  Total budget: 4.6 M€
- ΚΑΡΑΘΕΟΔΩΡΗ 2010(ΕΛΚΕ Π.Π.) «Συμπολυμερή του αλγινικού νατρίου εμβολιασμένα με πολύ(*N*-ισοπροπυλακρυλαμίδιο) ως θερμοπαχυντικά μέσα. Αξιοποίηση στη μεταφορά και απελευθέρωση φαρμάκων
  Total budget: 33.000 €

Recent Publications LSTM group

- Anastasiou A., E.K. Karahaliou, O. Alexiadis, V.G. Mavrantzas, "Detailed atomistic simulation of the nano-sorption and nano-diffusivity of water, tyrosol, vanillic acid and p-coumaric acid in single wall carbon nanotubes", J. Chem. Phys. 2013, 139, p. 164711.
- Stephanou P.S., V.G. Mavrantzas, "Quantitative predictions of the linear viscoelastic properties of entangled polyethylene and polybutadiene melts via modified versions of modern tube models on the basis of atomistic simulation data", J. Non-Newt. Fluid Mech. 2013, 200, p. 111.
- Alexiadis O., V.G. Mavrantzas, "All-atom molecular dynamics simulation of temperature effects on the structural, thermodynamic, and packing properties of the pure amorphous and pure crystalline phases of regioregular P3HT", Macromolecules 2013, 46, p. 2450.
- Qin J., S.T. Milner, P.S. Stephanou, V.G. Mavrantzas, "Effects of tube persistence length on dynamics of mildly entangled polymers", J. Rheology 2012, 56, p. 707.
- Brás A.R., R. Pasquino, T. Koukoulas, G. Tsolou, O. Holderer, A. Radulescu, J. Allgaier, V.G. Mavrantzas, W. Pyckhout-Hintzen, A. Wischnewski, D. Vlassopoulos, D. Richter, "Structure and Dynamics of Polymer Rings by Neutron Scattering: Breakdown of the Rouse Model", Soft Matter 2011, 7, p. 11169.
- Stephanou P.S., C. Baig, V.G. Mavrantzas,* "Toward an improved description of constraint release and contour length fluctuations in tube models for entangled polymer melts from detailed atomistic molecular dynamics simulation data", Macromol. Theory & Simul. 2011, 20, p. 752.
- Stephanou P.S., C. Baig, V.G. Mavrantzas, "Projection of atomistic simulation data for the dynamics of entangled polymers onto the tube theory: Calculation of the segment survival probability function and comparison with modern tube models", Soft Matter 2011, 7, p. 380.
- Baig C., V.G. Mavrantzas, H.C. Öttinger, "On Maxwell's Relations of Thermodynamics for Polymeric Liquids away from Equilibrium", Macromolecules 2011, 44, 640.

Recent Publications MacroEng group

- Responsive reversible hydrogels from associative "smart" macromolecules **C. Tsitsilianis,** *Soft Matter*, **6**, 2372-2388, (2010). (***invited review***).
- pH responsive self assemblies from A_n-core-(B-*b*-C)$_n$ heteroarm star block terpolymer bearing oppositely charged segments. Z. Iatridi and **C. Tsitsilianis*** *Chem. Commun.* 47, 5560-5562, (2011).
- pH-Responsive Hydrogel/Liposome Soft Nanocomposites For Tuning Drug Release. M.-T. Popescu, S. Mourtas, G. Pampalakis, S. G. Antimisiaris, and **C. Tsitsilianis*** *Biomacromolecules* **12**, 3023-3030, (2011).
- pH responsive MWCNT/star terpolymer nanohybrids. Z. Iatridi and **C. Tsitsilianis*** *Soft Matter*, **9**, 185-193, (2013).
- **W**ater-soluble stimuli responsive star-shaped segmented macromolecules. Z. Iatridi and **C. Tsitsilianis** * *Polymers* **3**, 1911-1933 (2011) (***invited review***)
- Three different types of physical gels arisen from a common rtriblock copolyme precursor: the case of ionomer gel. N. Stavrouli, Z. Iatridi, T. Aubry and **C. Tsitsilianis*** *Polym. Chem.* **4**, 2097-2105 (2013).
- Multicompartmental microcapsules from Star copolymer micelles. I. Choi, S. T. Malak, W. Xu, W. T. Heller, **C. Tsitsilianis** and V. V. Tsukruk* *Macromolecules* **46**, 1425-1436 (2013).
- Controlled Delivery of Functionalized Gold Nanoparticles by pH-Sensitive Polymersomes. M.-T. Popescu and **C. Tsitsilianis*** *ACS Macro Letters* **2**, 222-225 (2013).
- Perfect mixing of immiscible macromolecules at fluid interfaces. S. S. Sheiko*, J. Z. Zhou, J. Arnold, D. Neugebauere, K. Matyaszewski, **C. Tsitsilianis**, V. V. Tsukruk, J-M. Y. Carrillo, A. V. Dobrynin and M. Rubinstein *Nature Mater.* **12**, 735-740, (2013).

Recent Publications WsPol group

- "Thermoresponsive Sodium Alginate-*g*-Poly (*N*-Isopropylacrylamide) Copolymers III. Solution Properties" C. N. Cheaburu, O.N. Ciocoiu, **G. Staikos**, C. Vasile, *J. Appl. Polym. Sci*. 127 (5), 3340-3348 (2013).
- ""Hybrid material based on ST-AA photonic crystal core and ZnO particle shell" A. Mocanu, E. Rusen, C. Cincu, **G. Staikos** *Coll. Polym. Sci.* 290 (18), 1949-1954 (2012).
- ""Microstructure of Polyelectrolyte Nanoaggregates Studied by Fluorescence Probe Method" Vasilescu M., Angelescu D. G., Bandula R., **Staikos G**., *J. Fluor.* 21 (6), 2085-2091 (2011).
- "Characterization of the Core-Shell Nanoparticles Formed as Soluble Hydrogen-bonding Interpolymer Complexes at Low pH" M. Sotiropoulou, F. Bossard, E. Balnois, J. Oberdisse and **G. Staikos ,** *Langmuir* 23, 11252-11258 (2007).
- "Characterization of the Soluble Nanoparticles Formed through Coulombic Interaction of Bovine Serum Albumin with Anionic Graft Copolymers at Low pH" E. Serefoglou, J. Oberdisse and **G. Staikos ,** *Biomacromolecules* 8, 1195-1199 (2007).
- "Water-Soluble Hydrogen-Bonding Interpolymer Complex Formation between Poly(ethyleneglycol) and Poly(acrylic acid) Grafted with Poly(2-acrylamido-2-methylpropanesulfonic acid)" P. Ivopoulos, M. Sotiropoulou, G. Bokias and **G. Staikos ,** *Langmuir* 22, 9181-9186 (2006).
- "Water-Soluble Complexes through Coulombic Interactions between Bovine Serum Albumin and Anionic Polyelectrolytes Grafted with Hydrophilic Nonionic Side Chains" M. Sotiropoulou, G. Bokias and **G. Staikos ,** *Biomacromolecules* 6, 1835 (2005).

Some statistics

	total	2008-13
No of papers	234	60
No of chapters	19	10
No of conferences	308	76
PhD awarded	18	4
MSc awarded	25	11

Average IF of peer reviewed Journals (2008-2013) 4.34

Total Citations 5769