

Macromolecular Chemistry & Responsive Polymers

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Main expertise fields

- New approaches for the synthesis of advanced thermoplastics, thermosets and elastomers with targeted properties
- Chemistry, physics and transport behaviour of charged (macromolecular) systems such as ionic liquids and polyelectrolytes
- Physics, structure and dynamics of polymers and nanocomposites, and associated multiscale modelling and strometric simulations
- Elastic and inelastic x-ray and neutron scattering techniques
- Contact mechanics, adhesion, friction, and surface interactions
- Mechanics of fracture, failure and fatigue of polymeric materials
- Additive manufacturing, 3D/4D printing and polymer processing

Research challenges

- Creation of advanced organic materials for actuators, energy storage, sorption, transport and sensing applications
- Application of advanced polymer chemistry and engineering approaches to generate high performance polymers and elastomers
- Development of novel computational approaches to better describe single and multiphase polymer melts and solutions and their interactions with nanoparticles
- Understanding, prediction and design of nanocomposite structure, viscoelastic, mechanical and tribological performance and transport behaviour
- Utilization of printing and additive manufacturing as a means of processing novel high performance macromolecular materials

Application areas

- Additive manufacturing
- Electrochemical energy storage
- Gas sorption and gas separation
- High-performance polymeric materials
- Sensing, actuation and energy generation
- Tire compound and reinforcement engineering

Main assets

- DISAFERAC** (ongoing)
 - Novel polyelectrolytes for energy storage
- Goodyear-LIST partnership (ongoing)
 - Synthesis of high performance polymeric materials for tires
- VISCOMANO** (ongoing)
 - Physics of ionic polymer nanocomposites
- COATHIN**
 - Liquid-assisted Nanopulsed Plasma Deposition of Multifunctional Coatings with Interpenetrating Hydrogel Networks
- InterBATT
 - Next generation all-solid-state Li-Sulfur Battery
- Other assets (academic & industrial)

Equipment

- High Performance Computing
- Specific glassware for moisture and air sensitive chemistry
- Schlenk lines
- High pressure glass reactors with working temperatures from -20 to +200°C
- Glassware for monomers and polymers synthesis
- Argon glove box
- Anhydrous solvents circulation apparatus
- Vacuum ovens and bells
- Baini glass drying apparatus (allow to dry samples and transfer them directly into the glove box without contact with atmosphere)
- Milli-Q water purification system
- 1200 Infinity gel permeation chromatograph with an integrated RI detector
- 1260 Infinity 8 gel permeation chromatograph with triple detectors (RI, Visc and Light Scattering)
- Viscometers with various capillary diameters and thermostat
- Molau VSP potentiostat/galvanostat
- Coin cell 2032 battery press
- Automatic film applicator
- Freeze dryer for organic solvents

Selected publications

- Shaplov, A. S.; Marcella, R.; Mecerreyes, D. *Recent Advances in Ionogel Polymer Electrolytes Based on Poly(ionic Liquids)*. *Electrochimica Acta* 2015, 175, 18-34.
- Pozzerelli, L.; Shaplov, A. S.; Salsamendi, M.; Nair, J. R.; Vygodski, Y. S.; Mecerreyes, D.; Gerbaldi, C. *Single-Ion Thin-Layer Copoly(ionic Liquids) on Electrodes for All-Solid-State Lithium Batteries*. *ACS Appl. Mater. Interfaces* 2016, 8 (16), 10350-10359.
- Pozzerelli, L.; Abouadze, M. A.; Rubatat, L.; Nair, J. R.; Shaplov, A. S.; Gerbaldi, C.; Mecerreyes, D. *Single-Ion Thin-Layer Copolymer Electrolytes Based on Poly(ethylene Oxide) and Methacrylate Sulfonamide Blocks for Lithium Metal Batteries*. *Journal of Power Sources* 2017, 364, 191-199.
- Pankratov, D. O.; Lozinskaya, E. I.; Vlasov, P. S.; Aubert, P.-H.; Plesse, C.; Vidal, F.; Vygodski, Y. S.; Shaplov, A. S. *Synthesis of Novel Families of Conductive Cationic Poly(ionic Liquids) and Their Application in All-Polymer Flexible Pseudo-Supercapacitors*. *Electrochimica Acta* 2018, 281, 777-788.
- Pankratov, D. O.; Lozinskaya, E. I.; Vlasov, P. S.; Aubert, P.-H.; Plesse, C.; Vidal, F.; Vygodski, Y. S.; Shaplov, A. S. *Synthesis of Novel Families of Conductive Cationic Poly(ionic Liquids) and Their Application in All-Polymer Flexible Pseudo-Supercapacitors*. *Electrochimica Acta* 2018, 281, 777-788.
- Binkkattar, M.; Lozinskaya, E. I.; Pankratov, D. O.; Vygodski, Y.; Schmidt, D. F.; Shaplov, A. S.; Schenker, M. *Influence of Cationic Poly(ionic Liquid) Architecture on the Ion Dynamics in Polymer Gel Electrolytes*. *J. Phys. Chem. C* 2019, 123 (21), 13225-13235.
- Gouveia, A. S. L.; Soares, B.; Simões, S.; Antozov, D. Y.; Lozinskaya, E. I.; Sarmento, B.; Shaplov, A. S.; Marmuth, J. M. *Ionogels with Novel Substituted Cationic Thermotropic Liquid Crystals*. *Thermotropic Liquid Crystals: Characterization and Properties*. *Int. J. Phys. Chem.* 2019, 59 (9), 852-865.
- Nürnberg, P.; Lozinskaya, E. I.; Shaplov, A. S.; Schenker, M. U. *Cooperation of a Novel Supramolecular Ionogel with a Solid-Liquid Electrolyte*. *J. Phys. Chem. B* 2020, 124 (5), 863-870.
- Gouveia, A. S. L.; Makabi, E.; Lozinskaya, E. I.; Shaplov, A. S.; Tomé, L. C.; Marmuth, J. M. *Poly(ionic Liquid)/Ionic Liquid Membranes with Fluoropolymer Derived Anions: Characterization and Biophysics Separation*. *ACS Sustainable Chem. Eng.* 2020, 8 (18), 7087-7096.
- Khan, M. S.; Karantzas, A. V.; Ohta, T.; Cai, Q. *The Effect of Polymer Organic Solvents and Aqueous Salts on Sodium Ion Storage in Cyclized Carbon Nanotubes*. *Phys. Chem. Chem. Phys.* 2019, 21 (41), 22732-22733.
- Karantzas, A.; Composto, R. J.; Wiley, K. I.; Krogger, M.; Clarke, N. *Modeling of Entangled Polymer Diffusion in Melts and Nanocomposites*. *Adv. Polym. Sci.* 2019, 21 (5), 876.
- Karantzas, A.; Composto, R. J.; Wiley, K. I.; Clarke, N. *Nanosecond Diffusion in Polymer Nanocomposites by Molecular Dynamics Simulations*. *Macromolecules* 2019, 52 (6), 2513-2520.
- Vasilekio, I.; Todorovskov, V.; Saptsiankova, M.; Stöckhert, K. W.; Petry, F.; Westermann, S.; Henning, G. *Modeling of Dynamic-Mechanical Behaviour of Reinforced Elastomers Using a Multiscale Approach*. *Polymer* 2016, 87, 356-365.
- Schwarz, G. A.; Ortega, J.; Meyer, M.; Skjær, N. A.; Shi, C.; Westermann, S.; Cerveny, S. *Extended Adam-Gibbs Approach to Describe the Segmental Dynamics of Cross-Linked Miscible Rubber Blends*. *Macromolecules* 2018, 51 (5), 1741-1747.
- Bastarriz-Geni, B.; Hämäläinen, M.; Kjøper, F.; Valenčič, J. L.; Westermann, S.; Henning, G. *Segmental Segmental Order: A Simplified Approach for Solid-State Rubbers Considering Segmental Fluctuations and Intersegmental Interactions*. *Macromolecules* 2018, 51 (5), 2016-2028.
- Staropoli, M.; Gerstner, D.; Szucki, M.; Velhies, G.; Düez, B.; Westermann, S.; Lemble, D.; Pyschok-Hintzen, W. *Structural Softening Functions for Silica-Filled Rubbers under Different Types of Strain*. *ChemPhysChem* 2019, 20 (1), 9735-9745.
- Staropoli, M.; Gerstner, D.; Radulovic, A.; Szucki, M.; Düez, B.; Westermann, S.; Lemble, D.; Pyschok-Hintzen, W. *Decoupling the Contributions of ZnO and Silica to the Characterization of Industrially Mixed Filled Rubbers by Combining Small Angle Neutron and X-Ray Scattering*. *Polymers* 2020, 12 (3), 502.

Partners

University of Cergy-Pontoise, University of Maastricht, University of the Basque Country Donostia - San Sebastián, University of Lyon, University of Lisbon, ETH Zürich, University of Mons, Goodyear Tire & Rubber Company

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