RESEARCH GROUP

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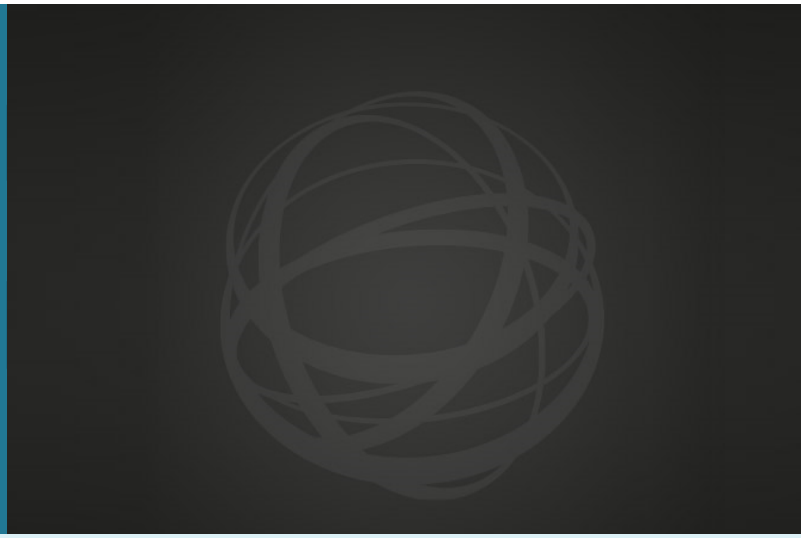
Macromolecular Chemistry & Responsive Polymers

The Macromolecular Chemistry and Responsive Polymers group utilizes new synthetic approaches and advanced processing, informed by polymer physics, to realize and control the response of novel functional polymeric materials and nanocomposites.



The Macromolecular Chemistry and Responsive Polymers group utilizes new synthetic approaches and advanced processing, informed by polymer physics, to realize and control the response of novel functional polymeric materials and nanocomposites.

Main expertise fields

- New approaches for the synthesis of advanced thermoplastics, thermosets and elastomers with targeted properties
- Chemistry, physics and transport behaviour of charged (macro)molecular systems such as ionic liquids and polyelectrolytes
- Physics, structure and dynamics of polymers and nanocomposites, and associated multiscale modelling and atomistic 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

1. DISAFECAP (ongoing)
   - Novel polyelectrolytes for energy storage
- Goodyear-LIST partnership (ongoing)
   - Synthesis of high performance polymeric materials for tires
- VISIONNANO (ongoing)
   - Physics of ionic polymer nanocomposites
- COATIHN
   - 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 +200oC
- Glassware for monomers and polymers synthesis
- Argon glove box
- Anhydrous solvents circulation apparatus
- Vacuum ovens and bells
- Buchi 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 II gel permeation chromatographs with triple detectors (RI, Visco and Light Scattering)
- Viscometers with various capillary diameters and thermostat
- Mobile VSP potentiostat/galvanostat
- Coin cell 2032 battery press
- Automatic film applicator
- Freeze dryer for organic solvents

Selected publications

- Shaplov, A. S.; Marcilla, R.; Mecerreyes, D. Recent Advances in Innovative Polymer Electrolytes Based on Poly(Ionic Liquids). *Electrochimica Acta* 2015, *175*, 18–34.
- Porcarelli, L.; Shaplov, A. S.; Salsamendi, M.; Nair, J. R.; Vygodskii, Y. S.; Mecerreyes, D.; Gerbaldi, C. Single-Ion Block Copolytionic Liquids as Electrolytes for All-Solid State Lithium Batteries. *ACS Appl. Mater. Interfaces* 2016, *8* (16), 10350–10359.
- Porcarelli, L.; Aboudzadeh, M. A.; Rubatat, L.; Nair, J. R.; Shaplov, A. S.; Gerbaldi, C.; Mecerreyes, D. Single-Ion Triblock Copolymer Electrolytes Based on Poly(Ethylene Oxide) and Methacrylic Sulfonamide Blocks for Lithium Metal Batteries. *Journal of Power Sources* 2017, *364*, 191–199.
- Ponkratov, D. O.; Lozinskaya, E. I.; Vlasov, P. S.; Aubert, P.-H.; Plesse, C.; Vidal, F.; Vygodskii, Y. S.; Shaplov, A. S. Synthesis of Novel Families of Conductive Cationic Polytionic Liquids and Their Application in All-Polymer Flexible Pseudo-Supercapacitors. *Electrochimica Acta* 2018, *281*, 777–788.
- Ponkratov, D. O.; Lozinskaya, E. I.; Vlasov, P. S.; Aubert, P.-H.; Plesse, C.; Vidal, F.; Vygodskii, Y. S.; Shaplov, A. S. Synthesis of Novel Families of Conductive Cationic Polytionic Liquids and Their Application in All-Polymer Flexible Pseudo-Supercapacitors. *Electrochimica Acta* 2018, *281*, 777–788.
- Brinkkötter, M.; Lozinskaya, E. I.; Ponkratov, D. O.; Vygodskii, Y.; Schmidt, D. F.; Shaplov, A. S.; Schönhoff, M. Influence of Cationic Polytionic 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.; Antonov, D. Y.; Lozinskaya, E. I.; Saramago, B.; Shaplov, A. S.; Marrucho, I. M. Ionic Liquid with Silyl Substituted Cation: Thermophysical and CO 2 /N 2 Permeation Properties. *Isr. J. Chem.* 2019, *59* (9), 852–865.
- Nürnberg, P.; Lozinskaya, E. I.; Shaplov, A. S.; Schönhoff, M. Li Coordination of a Novel Asymmetric Anion in Ionic Liquid-in-Li Salt Electrolytes. *J. Phys. Chem. B* 2020, *124* (5), 861–870.
- Gouveia, A. S. L.; Malcaitè, E.; Lozinskaya, E. I.; Shaplov, A. S.; Tomé, L. C.; Marrucho, I. M. Polytionic Liquid-Ionic Liquid Membranes with Fluorosulfonyl-Derived Anions: Characterization and Biohydrogen Separation. *ACS Sustainable Chem. Eng.* 2020, *8* (18), 7087–7096.
- Khan, M. S.; Karatrantos, A. V.; Ohba, T.; Cai, Q. The Effect of Different Organic Solvents and Anion Salts on Sodium Ion Storage in Cylindrical Carbon Nanopores. *Phys. Chem. Chem. Phys.* 2019, *21* (41), 22722–22731.
- Karatrantos, A.; Composto, R. J.; Winey, K. I.; Kröger, M.; Clarke, N. Modeling of Entangled Polymer Diffusion in Melts and Nanocomposites: A Review. *Polymers* 2019, *11* (5), 876.
- Karatrantos, A.; Composto, R. J.; Winey, K. I.; Clarke, N. Nanorod Diffusion in Polymer Nanocomposites by Molecular Dynamics Simulations. *Macromolecules* 2019, *52* (6), 2513–2520.
- Ivaneiko, I.; Toshchevikov, V.; Saphiannikova, M.; Stöckelhuber, K. W.; Petry, F.; Westermann, S.; Heinrich, G. Modeling of Dynamic-Mechanical Behavior of Reinforced Elastomers Using a Multiscale Approach. *Polymer* 2016, *82*, 356–365.
- Schwartz, G. A.; Ortega, L.; Meyer, M.; Isitman, N. A.; Sill, 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.
- Basterra-Beroiz, B.; Rommel, R.; Kayser, F.; Valentin, J. L.; Westermann, S.; Heinrich, G. Resisting Segmental Order: A Simplified Approach for Sulfur-Cured Rubbers Considering Junction Fluctuations and Entanglements. *Macromolecules* 2018, *51* (5), 2076–2088.
- Staropoli, M.; Gerstner, D.; Sztucki, M.; Vehres, G.; Duez, B.; Westermann, S.; Lenoble, D.; Pyckhout-Hintzen, W. Hierarchical Scattering Function for Silica-Filled Rubbers under Deformation. Effect of the Initial Cluster Distribution. *Macromolecules* 2019, *52* (24), 9735–9745.
- Staropoli, M.; Gerstner, D.; Radulescu, A.; Sztucki, M.; Duez, B.; Westermann, S.; Lenoble, D.; Pyckhout-Hintzen, W. Decoupling the Contributions of ZnO and Silica in 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 MÃ¼nster, University of the Basque Country Donostia - San SebastiÃin, University of Lyon, University of Lisbon, ETH ZÃ¼rich, University of Mons, Goodyear Tire & Rubber Company

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