

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

- DISAFFEAL** (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 chromatographs 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.
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- Gouveia, A. S. L.; Makabi, E.; Loznitskaya, E. I.; Shaplov, A. S.; Tomé, L. C.; Marmutho, 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.; Oñate, T.; Cui, 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. *Simulation of Entangled Polymer Diffusion in Melts and Nanocomposites*. *Adv. Polym. Sci.* 2019, 21 (5), 876.
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- Bastarratzen, B.; Hämäläinen, M.; Kjøper, F.; Valenčič, J. L.; Westermann, S.; Henrich, G. *Segmental Dynamics of a Ring-Closed Polymer Containing a Specific Functional Group*. *Macromolecules* 2018, 51 (5), 2016-2028.
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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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