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Supervisor	**Period**	**Funding**
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Multiscale modelling of polymeric production processes for sustainable electrical energy production and storage

Aim

The aim is to develop a kinetic model for the production of polyelectrolytes to be used in photovoltaic cells and electrical batteries, by relying on polymer reaction engineering principles. The model will support the design and optimization of novel and existing polymer production processes for solar energy harvesting and storage, by providing novel insights in micro- and mesoscale phenomena and predicting material properties/performance.

Justification

An important societal challenge is meeting the ever increasing energy consumption with renewable or sustainable energy sources using technological advances in the field. For example, electrical energy can be sustainably produced by harvesting solar energy via photovoltaic cells, converting into electrical energy and storing in electrical batteries. High-tech polymeric materials are important candidates for both organic photovoltaic cells and electrical batteries, avoiding the use of rare-earth metals in inorganic solar cells. In the past decades, the photon efficiency of organic photovoltaic cells has approached the efficiency of existing commercialized inorganic photovoltaic cells, at least in laboratory conditions. However, large efficiency gains are expected when optimizing micro- and mesoscale process parameters. Similarly, electrical batteries based on polyelectrolytes (see Figure) are expected to achieve superior energy storage compared to existing non-polymers based technology.

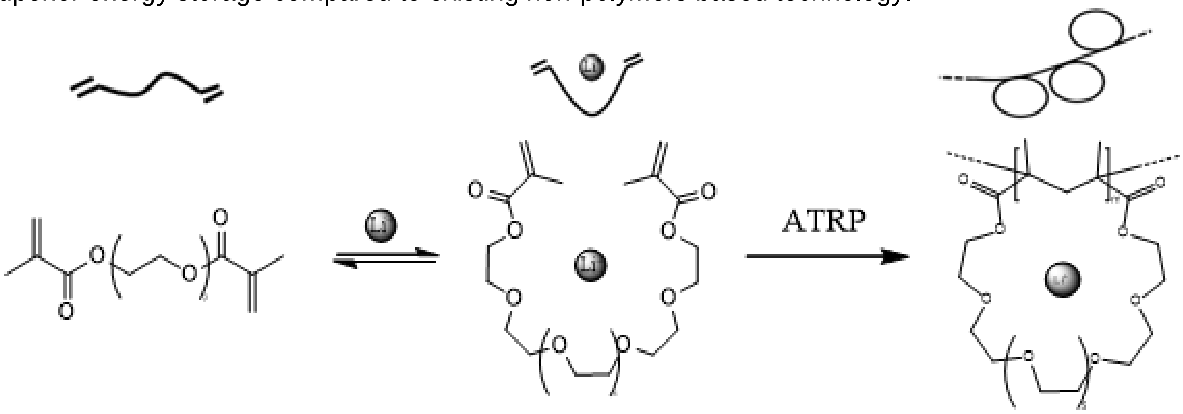

Figure: Atom transfer radical polymerization products as "molecular diffusion pipes" to provide mobility for Li^+ in electrical batteries.

Program

1. Literature study of micro- and mesoscale phenomena for polyelectrolytes (*e.g.* poly(vinylidene fluoride) (PVDF) and poly(phenylenevinylene) (PPV)) in photovoltaic cells and electrical batteries.
2. Modeling the synthesis of polyelectrolyte(s) (networks) and predicting microstructural properties.
3. Designing/conducting experiments in collaboration with current and new (inter)national academic/industrial partners (UMons, UHasselt, KIT, *etc.*).
4. Correlating microstructural properties with material properties (*e.g.* electrical conductivity).
5. Benchmarking and applying the model over a wide range of industrially relevant conditions.
6. Publishing in leading journals on chemical engineering and polymer (materials) science.