A novel tool to support the characterization of polymer gels

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A key innovation goal for next-generation polymer synthesis is the improved microstructural control of complex macromolecular structures, *i.e.* 3D polymer gels. Such macromolecular precision control will facilitate the realization of high-tech applications such as the development of carriers for site-specific delivery of drugs, provided that they are sufficiently biocompatible. A challenge is the provision of 'ideal networks' with controlled/homogeneous composition and well-defined pore size distribution, since it can be expected that thermal, mechanical and swelling properties are then improved. Important as well is the exact positioning of functional groups within the network as this influences drug-network interactions. A bottleneck is however the limited understanding of the effect of reaction conditions on the final macroscopic properties of polymer gels and the product performance.

Therefore in the present work a novel modeling tool is developed, starting from previous developments for linear polymer systems [1], allowing a complete characterization of the evolution of the polymer microstructure of individual macromolecules during network formation. Model validation is currently performed based on network synthesis considering the para-fluoro-thiol reaction (PFTR), a nucleophilic substitution reaction between a pentafluorophenyl group and a thiol derivative [2,3]. Dedicated experimental analysis has been applied to tune the model parameters and a good agreement between experimental and modeled data is obtained. In the long term, the tool can be applied for model-based design to identify highly efficient protocols for the synthesis of hydrogels and the research will therefore offer unique opportunities for a broad range of enhanced (biomedical) applications.

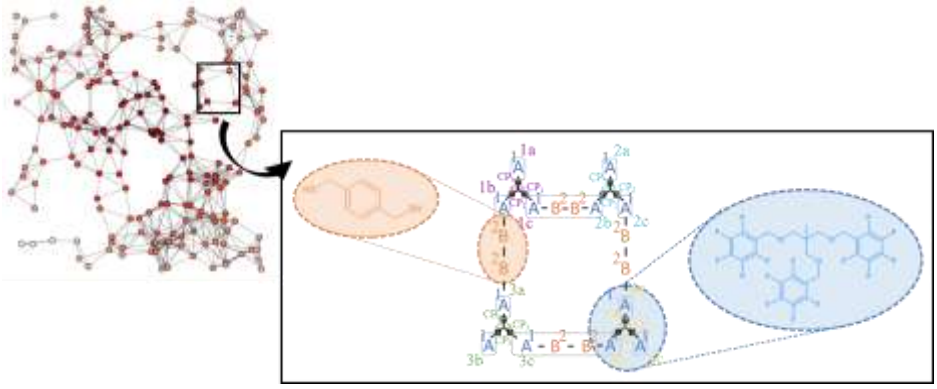

Figure 1. Representation of a pore in PFTR system

[1] D. R. D'hooge, P. H. M. Van Steenberge, M.-F. Reyniers, G. B. Marin *Prog. Polym. Sci.* **2016**, 58, 59-89.
[2] F. Cavalli, H. Mutlu, S. O. Steinmueller, L. Barner *Polym. Chem.* **2017**, 8, 3778-3782.
[3] G. Delaittre, L. Barner *Polym. Chem.* **2018**, 9, in press.