

<p>Physical Chemistry <b>P1</b></p> <p style="text-align: center;"><b>Molecular Switches with Logic Functions</b></p> <p style="text-align: center;"><u>Uwe Pischel</u></p> <p style="text-align: center;">CIQSO – Center for Research in Sustainable Chemistry, University of Huelva, Campus de El Carmen, s/n, E-21071 Huelva, Spain</p> <p>The application of (photo)chemical switching in the sense of the principles of Boolean logic has created considerable attention in recent years.<sup>1,2</sup> Indeed, it is a beguiling idea to use molecules as nano-building-blocks for the realization of functions that we know otherwise only from conventional computing based on silicon circuitry. The field has reached a rather high level of maturity during the last 20 years. However, it has to be seen with a certain portion of realism that the final objective of a powerful molecular computer is still very distant. On the other hand, while the bottleneck problems are identified at the moment, molecular logic is developing in many other directions, with implications for intelligent sensing, drug activation and delivery, and smart materials.<sup>3</sup></p> <p>This presentation deals with the basics and applications of molecular logic. Emphasis will be given to our own works that are centered in the development of chemically and photochemically switchable logic systems that can be read out through their fluorescence properties.<sup>4-7</sup></p> <p>[1] U. Pischel, <i>Angew. Chem. Int. Ed.</i> <b>2007</b>, <i>46</i>, 4026.  [2] J. Andréasson, U. Pischel, <i>Chem. Soc. Rev.</i> <b>2010</b>, <i>39</i>, 174.  [3] U. Pischel, J. Andréasson, D. Gust, V. F. Pais, <i>ChemPhysChem</i> <b>2013</b>, <i>14</i>, 28.  [4] R. Ferreira, P. Remón, U. Pischel, <i>J. Phys. Chem. C</i> <b>2009</b>, <i>113</i>, 5805.  [5] U. Pischel, V. D. Uzunova, P. Remón, W. M. Nau, <i>Chem. Commun.</i> <b>2010</b>, <i>46</i>, 2635.  [6] V. F. Pais, P. Remón, D. Collado, J. Andréasson, E. Pérez-Inestrosa, U. Pischel, <i>Org. Lett.</i> <b>2011</b>, <i>13</i>, 5572.  [7] P. Remón, M. Bälter, S. M. Li, J. Andréasson, U. Pischel, <i>J. Am. Chem. Soc.</i> <b>2011</b>, <i>133</i>, 20742.</p>	<p>Polymers, Colloids Interfaces <b>P2</b></p> <p style="text-align: center;"><b>Ti(IV) and Zr(IV) N-heterocyclic carbene complexes: synthesis, reactivity and use of them in the controlled ring-opening polymerization of <i>rac</i>-lactide and trimethylene carbonate</b></p> <p style="text-align: center;">Charles Romain,<sup>a</sup> Stéphane Bellemin-Laponnaz,<sup>a</sup> Ralf Dümpelmann,<sup>b</sup> Pascal Steffanut,<sup>b</sup> Samuel Dagorne<sup>a</sup></p> <p style="text-align: center;"><sup>a</sup>IPCMS and Institute of Chemistry of Strasbourg, University of Strasbourg – CNRS; <sup>b</sup>Clariant Products (Switzerland) Ltd</p> <p>Despite their potential interest in catalysis, high-oxidation-state and oxophilic transition metal complexes bearing NHC ligands have been much less studied as these complexes are expected to be less stable due to an easier M-C<sub>carbene</sub> bond dissociation in such species. Thus, for the most part, the suitability of such species for catalysis remains to be addressed.</p> <p>We have become interested in the synthesis of robust NHC-containing group 4 metal complexes for their subsequent use in catalysis polymerization of renewable-resource-derived monomers such as cyclic esters and carbonates (lactide, LA, and trimethylene carbonate, TMC). To this purpose, we have developed a novel family of tridentate bis-aryloxy-NHC dianionic chelating ligands in which the NHC moiety is positioned as a central donor for coordination to group 4 metal centers [1]. Remarkably, the synthesized group 4 NHC metal complexes exhibit an exceptional robustness and, most notably, mediate the highly controlled and stereoselective ring-opening polymerization of <i>rac</i>-LA for the production of heterotactic PLA (as well as associated LA/TMC co-polymers) [2-4]. All these aspects will be thoroughly discussed in the present lecture.</p> <p>[1] Romain, C., Miqueu, K., Sotiropoulos, J.-M., Bellemin-Laponnaz, S., Dagorne, S. <i>Angew. Chem. Int. Ed.</i> <b>2010</b>, <i>49</i>, 2198-2201.  [2] Romain, C., BreLOT, L., Bellemin-Laponnaz, S., Dagorne, S. <i>Organometallics</i> <b>2010</b>, <i>29</i>, 1191-1198.  [3] Romain, C., Dagorne, S., Bellemin-Laponnaz, S., Steffanut P. WO2012076140 (A1) (2012-06-14)  [4] Romain, C., Heinrich B, Bellemin-Laponnaz, S., Dagorne S. <i>Chem. Commun.</i> <b>2012</b>, <i>48</i>, 2213-15.</p>
<p>Medicinal Chemistry Chemical Biology <b>P3</b></p> <p style="text-align: center;"><b>30 Years at the Interface between Science and Technology</b></p> <p style="text-align: center;">Klaus Müller</p> <p style="text-align: center;">F. Hoffmann-La Roche AG, CH-4070 Basel, Switzerland</p> <p>With the publication of the first X-ray crystal structures of bacterial dihydrofolate reductases in the early 1980's, Roche decided to embark on structure-based molecular design. It was a pioneering decision with many risks and challenges. This commitment required the concurrent implementation of protein X-ray crystal structural analysis within the confines of pharmaceutical industry. This in turn provoked an early entry into bioinformatics. All three research areas started at Roche in the 1980's, at times when strong cautions were voiced against such activities in industry. Much research with technology development and interactive collaboration between experts of different disciplines were required to bring these endeavors to fruition. All three areas now constitute firm pillars of modern pharmaceutical research.</p> <p>In the 1990's, structure-based research was complemented by high-throughput screening of large compound libraries. Challenging requirements for sample storage/retrieval and ultra-HT screening again prompted innovative developments. It was also the time of miniaturization and automation in the field of physicochemical property analytics. Their successful development in combination with improved methods for measuring pharmacologically relevant <i>in vitro</i> compound properties resulted in a paradigm shift of pharmaceutical research from linear to multi-dimensional lead optimization.</p> <p>During the subsequent decade, continuous explorations of novel concepts in medicinal chemistry, in terms of molecular structure and property, resulted in the discovery of oxetane, compact scaffolds, and partially fluorinated alkyl groups as potentially interesting property-modulating units.</p> <p>In all these activities, intense collaborations with excellent colleagues have been crucial for success. This account will highlight their contribution.</p>	