

MOLECULAR DYNAMICS SIMULATIONS OF SEQUENCE-DEFINED OLIGOMERS FOR CATALYSIS

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Nature has the amazing ability to achieve a perfect control of monomer sequence in biological macromolecules. This microstructural precision leads to sophisticated structures with remarkable functions such as catalysis, molecular recognition, and information storage¹. Inspired by the precision of biological macromolecules, the design of synthetic sequence-defined polymers constitutes an emerging topic of interest to generate materials with next-generation performances². Despite considerable progress on the control over the primary structure, the controlled folding and assembly of synthetic polymers into predetermined three-dimensional shapes have not been achieved so far.

Here we use computational chemistry approaches to decipher the structure and dynamics of sequence-defined oligomeric chains used for supported catalysis. These oligomers incorporate structuring groups and three functional moieties, *i.e.*, 2,2,6,6-tetramethyl-1-piperidinyloxy (TEMPO), N-methylimidazole (NMI) and pyridyltriazole (pyta)-Cu^I complex (pyta-Cu^I), for the selective oxidation of alcohols (Figure 1)³. The oligomeric chains under study differ by the monomer sequence and the number of molecular spacers between the catalytic moieties. In combination with experimental catalytic activity, our computational study brings insights into structure-activity relationships for targeted applications in catalysis.

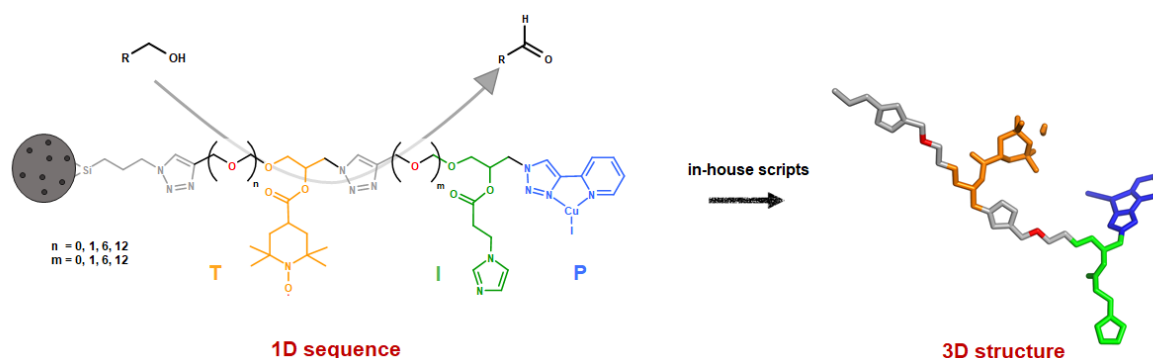


Figure 1: Sequence-defined oligomers with connecting fragments, molecular spacers of various lengths and three functional moieties, *i.e.*, TEMPO (T), N-methylimidazole (I), and pyridyltriazole-Cu^I complex (P) for the selective oxidation of alcohols.

References.

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