

**Evaluating the performance of early transition metal complexes in the preparation of disentangled ultra-high molecular weight poly(ethylene)**

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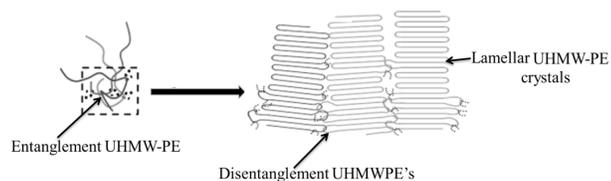
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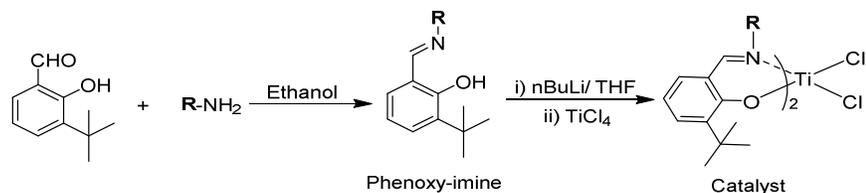
**Abstract**

A linear polyethylene with molecular weight larger than ~2-3 million g/mol can be defined as belonging to the class of ultra-high molecular weight poly (ethylene) s (UHMW-PE)<sup>1</sup>. However, UHMW-PE is difficult to process in the melt state, since the long-chains are highly entangled in the melt resulting in extremely high melt viscosity( Fig.1)<sup>1</sup>. Recently, it has been shown that UHMW-PE can be prepared in solution in a disentangled state using a soluble titanium Schiff base complex at low temperatures<sup>2</sup>.



**Figure 1.** Entangled and disentangled state in UHMW-PE.

Methodologies that provide predictable control over the product properties are highly desired in molecular and macromolecular synthesis. Greater fundamental understanding of factors that control chain growth and chain transfer will lead to strategies for a rational design of molecular catalyst for the preparation of UHMW-PE in a disentangled UHMWPE. The success of such methodologies will totally rely on the ligand choice and the ability to manipulate electronic and steric environment around the active center. We present herein an approach towards design of an early transition metal complex with apt balance of steric and electronic parameters that provide control over the relative rates of propagation and transfer. Synthesis of Schiff's base metal complexes (Scheme 1), where R is either a cycloalkyl or aryl group and their efficacy for the preparation of UHMW-PE will be presented.



**Scheme 1.** Synthesis of early transition metal complexes

**References**

1. P. Smith, P.J. Lemstra, J.P.L. Pijpers, and A.M. Kiel, *Colloid. Polym. Sci.*, 259, 11 (1981); US4344908 A (1982)
2. Saeid Talebi, Rob Duchateau, Sanjay Rastogi, Joachim Kaschta, Gerrit W. M. Peters, Piet J. Lemstra., *Macromolecules.*, 2010, 43, 2780–2788