

## Ziegler-Natta PP Catalysts Demystified

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Isotactic polypropylene (i-PP) is the second large-volume polymer on the market after polyethylene (PE). The current production of 60 MT/y is almost entirely based on MgCl<sub>2</sub>-supported Ti-based catalysts of Ziegler-Natta (ZN) type. The active forms of these systems are obtained by the interaction of a MgCl<sub>2</sub>/TiCl<sub>4</sub>/ID precatalyst (ID = Internal [electron] Donor) with an AlR<sub>3</sub>/ED cocatalyst (ED = External [electron] Donor).<sup>1,2</sup>

It is generally agreed that the active sites are inherently chiral alkylated Ti(III) species with donor molecules at non bonded contact, but their number and structure(s) are uncertain. Throughout decades of experimental and theoretical investigations, practically all possible hypotheses (including of course contrasting ones) have been proposed. As a matter of fact, rather than coming up with novel ideas, what is really needed now is to carefully go through existing interpretations, and identify those that are compatible with the large amounts of experimental and computational data recently made available by HTE and HTC studies.

As will be shown in this talk, the conclusion of such an exercise is that it is indeed possible to define a picture of Ziegler-Natta catalysts for PP that convincingly addresses all questions of interest, including in the first place the number and structure of the active sites.

### General References

- (1) Cecchin, G.; Morini, G.; Piemontesi, F. In *Kirk-Othmer Encyclopedia of Chemical Technology* (5<sup>th</sup> Edition); Seidel, A., Ed; John Wiley & Sons: Hoboken (NJ), 2007; Vol. 26, pp. 502-554.
- (2) Moore, E. P. Jr., Ed. *Polypropylene Handbook*; Hanser-Gardner Publications: Cincinnati (OH), 1996.