

Molecular understanding of Cr-based Ethylene Polymerization Catalysts

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The Phillips polymerization catalysts are responsible for ca. 50% of the world production of high density polyethylene, but despite greater than 50% years of research both in academia and in industry, the structure of the active sites and the polymerization mechanism remain unknown.

Here, we will discuss how Surface Organometallic Chemistry(1) combined with the preparation of molecular analogues and the use of computational models can provide information about Phillips catalysts.(2)

(1) C. Copéret, A. Comas-Vives, M. P. Conley, D. Estes, A. Fedorov, V. Mougel, H. Nagae, F. Núñez-Zarur, P. A. Zhizhko *Chem. Rev.* **2016**, *16*, 323–421.

(2) a) M. P. Conley, M. F. Delley, G. Siddiqui, G. Lapadula, S. Norsic, V. Monteil, O. V. Safonova, C. Copéret *Angew. Chem. Int. Ed.*, **2014**, *53*, 187-1876. b) Delley, M.F.; Núñez-Zarur, F.; Conley, M, P.; Comas-Vives, A.; Siddiqi, G.; Norsic, S.; Monteil, V.; Safonova, O. V.; Copéret C. *Proc. Nat. Acad. Sci.* **2014**, *111*, 11624–11629. c) M. P. Conley, M. F. Delley, F. Núñez-Zarur, A. Comas-Vives, C. Copéret, *Inorg. Chem.* **2015**, *54*, 5065-5068. d) Copéret et al. unpublished results.