

Research Group no. 1

UNIVERSITA' DI NAPOLI FEDERICO II

STERESELECTIVE OLEFIN POLYMERIZATIONS

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Members: Vincenzo Busico, Michele Vacatello, Roberta Cipullo, Giovanni Talarico, Peter H. M. Budzelaar, Angela D'Amora, Maddalena D'Amore, Antonello Pastore, Christian Ehm, Luca Rongo, Yue Yu, Emanuele Breuza, Marina Trinchillo, Pasquale Cacace, Alessio Mingione, Enrichetta Villano, Alessia Napolitano, Natascia Napolitano, Antonio Vittoria.

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The group is actively involved in stereochemical and mechanistic investigations of Ziegler-Natta and related transition-metal-catalyzed olefin polymerizations. Heterogeneous TiCl_3 and $\text{MgCl}_2/\text{TiCl}_4$ catalysts, as well as homogeneous (metallocene and post-metallocene) ones are the objects of both fundamental and applied studies, in collaboration with a number of world-leading industrial companies and with the Dutch Polymer Institute (DPI). The toolkit includes state-of-the-art High Throughput Experimentation and High Throughput Computation platforms, with advanced integrated analytical tools.

Researchers of the group were the first to introduce, in the mid-'90s, high-field ^{13}C NMR in the microstructural analysis of propene homo- and copolymers, aimed at a correlation with their physical properties on the one hand, and on the other at a "fingerprinting" of the catalytic species. The unprecedented level of detail in the evaluations of (co)monomer sequence distributions, combined with the development of new and powerful matrix multiplication codes for their statistical analysis, has led to substantial advances in our understanding of both material properties and of reaction regio-, stereo- and chemoselectivity. Kinetic methods, including hydro-oligomerization and quenched-flow techniques, are also currently applied in the group.

The experimental results are routinely complemented with advanced computer modeling. Quantum Mechanics, when needed in combination with Molecular Mechanics, is used to test models of active species and to explain or – in some cases – predict the observed selectivities of monomer insertion and ratios between chain propagation and transfer.

Key words: catalysis, polymerization, polyolefins, Ziegler-Natta, High Throughput Experimentation, High Throughput Computation

Representative recent publications:

- Rocchigiani, L.; Busico, V.; Pastore, A.; Macchioni, A. *Dalton Trans.* **2013**, Adv. Article, DOI: 10.1039/c3dt00041a

- Busico, V. *MRS Bull.* **2013**, 38, 224-228.

- D'Amore, M.; Credendino, R.; Budzelaar, P.H.M.; Causá, M.; Busico, V. *J. Catal.* **2012**, 286, 103-110.

- Ciancaleoni, G.; Fraldi, N.; Cipullo, R.; Busico, V.; Macchioni, A.; Budzelaar, P. H. M. *Macromolecules* **2012**, 45, 4046–4053.

- Ciancaleoni, G.; Fraldi, N.; Budzelaar, P.H.M.; Busico, V.; Macchioni, A. *Organometallics* **2011**, 30, 3096-3105.

- Ciancaleoni, G.; Fraldi, N.; Budzelaar, P.H.M.; Busico, V.; Cipullo, R.; Macchioni, A. *J. Am. Chem. Soc.* **2010**, 132, 13651-13653.

- Macko, T.; Cutillo, F.; Busico, V.; Brüll, R. *Macromol. Symp.* **2010**, 298, 182-190.

SUPPLEMENTARY MATERIAL

Position of the components of the Research Groups

Name	Surname	Position *	Affiliation
Vincenzo	Busico	PO	Univ. Napoli Federico II and Dutch Polymer Institute (DPI)
Michele	Vacatello	PO	Università di Napoli "Federico II"
Roberta	Cipullo	PA	Università di Napoli "Federico II"
Giovanni	Talarico	PA	Università di Napoli "Federico II"
Peter H. M.	Budzelaar	VR	University of Manitoba (Canada)
Angela	D'Amora	RU (RTD)	Università di Napoli "Federico II"
Maddalena	D'Amore	PoD	Università di Napoli "Federico II"
Antonello	Pastore	PoD	Università di Napoli "Federico II" and DPI
Christian	Ehm	PoD	Università di Napoli "Federico II" and DPI
Luca	Rongo	PoD	Università di Napoli "Federico II" and DPI
Yue	Yu	PhD	Università di Napoli "Federico II"
Emanuele	Breuzza	PhD	Università di Napoli "Federico II" and DPI
Marina	Trinchillo	PhD	Università di Napoli "Federico II"
Pasquale	Cacace	T	Università di Napoli "Federico II"
Alessio	Mingione	T	Università di Napoli "Federico II" and DPI
Enrichetta	Villano	T	Università di Napoli "Federico II"
Alessia	Napolitano	T	Università di Napoli "Federico II"
Natascia	Napolitano	T	Università di Napoli "Federico II"
Antonio	Vittoria	T	Università di Napoli "Federico II" and DPI

*: PO = Full professor; PA = Associate professor; RU = University researcher; CO = contract; PoD = Postdoctoral fellows; RC = CNR staff or other Institutions Research; T = technician, VR = visiting researcher, S = student

Main Equipment

Type	Producer	Year of acquisition
Bruker Avance DRX 400 NMR	Bruker	2013
Bruker Avance III 400 NMR with high-temperature cryoprobe	Bruker	2012
ICP-OES 710	Agilent	2011
Dell PowerEdge Blade Server Cluster (180 cpu)	Dell	2010
Parallel Pressure Reactor PPR48	Freeslate	2010 (upgrade)
Core Module CM2	Freeslate	2008

Technical skills

- Organometallic chemistry
- Polymerization catalysis
- High Throughput Experimentation
- High Throughput Computation
- Microstructure Polymer Analysis