

# Dr. Giuseppe Milano CURRICULUM VITAE



**Date of Birth :** March 14<sup>th</sup> , 1970

**Place of Birth :** Napoli (NA), Italy

**Private Address :** Via Fortunato 55 Bis, 84084, Fisciano (Salerno), Italy

**Civil Satus :** Married

**Current Affiliation:** Modeling Lab for Nanostructure and Catalysis, Dipartimento di  
Chimica Università di Salerno I-84084 Fisciano (Salerno), Italy

**Current Position:** Assistant Professor of Chemistry

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## EDUCATION, SCIENTIFIC EXPERIENCE

### Appointments year by year

#### 1995

**March** Degree in Chemistry cum laude at the University of Napoli, supervisor Prof. Vincenzo Barone, working on the thesis titled: *“Developments and applications of computational strategies to study proton transfer reactions in excited states”*

**September** Grant from the University of Napoli to work in the laboratory directed by Prof. Robert Subra, University Joseph Fourier of Grenoble, France, for a stage in Theoretical chemistry methods applied to free radicals in bio-molecules.

**December** Military Service (conscription for 12 months, after three months with corporal rank) at South Italy Army Head Quarter in Naples.

#### 1999

**January** Ph.D. in Chemistry at the University of Salerno, supervisor Prof. Gaetano Guerra, working on the thesis titled: *“Study and characterization of Host-Guest interactions in nanoporous polymeric semicrystalline materials”*

**February** One year post-doctoral grant from Basell Polyolefins Italy, supervisors Prof. Gaetano Guerra and Dr. Luigi Resconi, on the project: *Theoretical studies on Ziegler-Natta catalysts for the polymerization of propene*

## 2000

**January** Two years post-doctoral position in the group directed by Prof. Gaetano Guerra on the project: *"Molecular separations by thermoplastic molecular sieves based on syndiotactic polystyrene"*

**September** Grant from Italian Research Council (CNR) *short term mobility for young researcher* to work as visiting scientist hosted in the Polymer Theory Group Directed by Prof. Dr. Kurt Kremer (Max-Planck-Institut für Polymerforschung Mainz, Germany) for molecular dynamics simulations studies about transport properties of polymers.

## 2002

**November** Assistant Professorship at University of Salerno

## 2003

**September** Research **Fellowship from Alexander von Humboldt Foundation**, at International University Bremen hosted by Prof. Dr. Florian Müller-Plathe title of the research project: *"Atomistic and Coarse Graining Simulation of Polymer Interfaces"*

## 2004

**September** Humboldt Fellowship Extension for three months

**December-up to now** Assistant Professor at University of Salerno, Modeling Lab for Nanostructures and Catalysis (MolNaC), Department of Chemistry.

## TEACHING EXPERIENCE

**2002-2003** Laboratory of Industrial Chemistry (University of Salerno, Chemistry, undergraduate level)

**2003-2004** Laboratory of Macromolecular Chemistry (University of Salerno, Chemistry, undergraduate level)

Ludwig Boltzmann Lectures :10 lessons for graduates and post-graduates at International University Bremen on Statistical Mechanics and its application to the study of Polymeric Materials. in collaboration with Prof. Müller-Plathe, Dr. D. Roccatano, Dr. S. Pal

Lessons on Coarse Grained Model of Polymers and Biopolymers

*At the Summer School on Advanced Modeling of Biological Function* organized at International University Bremen by Prof. Martin Zacharias

**2004-2005** Laboratory of Environmental Chemistry (University of Salerno ,Chemistry, undergraduate level )

Computational Chemistry Tutorials (International University Bremen, Chemistry, undergraduate and graduate level)

**2005-2006** Polymer Physical Chemistry (University of Salerno, Chemistry, senior undergraduate and graduate level)

Introduction to Scientific Programming (University of Salerno, Chemistry, undergraduate level)

**2006-2007** Polymer Physical Chemistry (University of Salerno, Chemistry, senior undergraduate and graduate level)

Introduction to Scientific Programming (University of Salerno, Chemistry, undergraduate level)

**2008-2009** Polymer Physical Chemistry (University of Salerno, Chemistry, senior undergraduate and graduate level)

Introduction to Scientific Programming (University of Salerno, Chemistry, undergraduate level)

## Scientific Interests

- Development of Multiscale Methods and Programs for Material Science Simulations
- Mesoscale Modeling, Coarse Grained Simulations of Macromolecular systems
- Development of Hybrid Particle Field approaches for Materials Simulations
- Density functional theory and *ab initio* calculations
- Combined Quantum Mechanics/Molecular mechanics techniques
- Nanomaterials. Polymer Nanoparticle Composites.
- Transport Properties in Polymers
- Mechanisms of olefins polymerizations.
- Host/guest interactions.

## Coordination of Research Projects

**2005** Coordinator of a Supercomputing Project in the Framework of CINECA (Italian National Supercomputing Center) and INSTM (Italian National Consortium for Science and Technology of Materials) agreement (11<sup>th</sup> edition): Duration 12 months

*Project title: "Polimeri Vinilici. Meccanismi di Polimerizzazione e Proprietà Fisiche: da Metodi Quantomeccanici a Modelli Coarse-Grained: un approccio multiscala"*

Status: Completed

**2006** Coordinator of a Supercomputing Project in the Framework of CINECA (Italian National Supercomputing Center) and INSTM (Italian National Consortium for Science and Technology of Materials) agreement (12<sup>th</sup> edition): Duration 12 months

*Project title: "Multiscale Modeling of Macromolecules: Synthetic Polymers and Biopolymers"*

Status Completed

**2008** National Coordinator of the PRISMA project (Innovative Research Projects in Material Science): Duration 24 months

*Project title: "Development and Application of Multiscale Methods for the Simulation of Polymer Nanoparticle Dispersions: From Electrons to Rheology"*

Status: Funded first startup

**2008** Co-responsible (together with Dr. Roccatano, German Partner at Jacobs University Bremen,) of the DFG project **RO 3571/3-1**

Duration 36 months

entitled: "*Study of Interaction mechanisms of block polymers with biological interfaces*"

Status: Funded first startup

**2008** JSPS Project in collaboration with Prof. Kawakatsu at Tohoku University Japan

entitled: "*Development of a particle/field hybrid multi-resolution approach to computational physics and material science*"

Status: Completed

## Languages

- Italian (mother tongue)
- English (fluent)
- German (good level) (G1 Certificate after an intensive course of 2 months at the Goethe Institut of Bremen, further practice in Germany)
- French (elementary level)

## Conference and Schools Organization

- Congresso dei Chimici Teorici di Espressione Latina CHITEL99  
Napoli 13-16 settembre 1999 (Organizing Committee member)
- 3rd Workshop on "Advances on Insertion Polymerisation"  
Ischia 11-13 settembre 2000 (Organizing Committee member)
- Advanced Modeling of Biological Function. Summer School  
International University Bremen August 2004 Germany (Organizing Committee member)
- 1<sup>st</sup> Workshop "Polymers in Nanotechnology"  
Salerno 27-28<sup>th</sup> September 2007 (International Representative member)

## Memberships and Consulting activity

- Consultant of STMicroelectronics for the Post Silicon Technology Division of the Company.
- Member of the association of Italian Humboldtians
- Permanent Member of the commission for PhD. in Chemistry at University of Salerno
- Member of the commission for PhD. in Chemical Engineering at University of Naples  
years 2006 and 2007.
- Member of AIM (Associazione Italiana Macromolecole) Italian Association of  
Macromolecular Science and Technology and of its newsletters editorial board.
- Member of INSTM (Consorzio Interuniversitario di Scienza e Tecnologia dei Materiali)  
Italian University Consortium of Material Science and Technologies.
- Founding Member and representative member for the Department of Chemistry of  
Nanomates (Interdipartimental Centre for Transdisciplinary Research in Nanoscience and  
Nanotechnology) at University of Salerno.
- Member of Mind Sh@re Community Finmeccanica (Multiscale Modeling Group)  
see: [http://www.finmeccanica.it/Holding/EN/Corporate/Tecnologia/Comunita\\_tecnologiche/index.sdo](http://www.finmeccanica.it/Holding/EN/Corporate/Tecnologia/Comunita_tecnologiche/index.sdo)

## Extracurricular Activities and Interests

- Philosophy (in particular Greek, Middle Age and Philosophy of Science).
- History (in particular Greek, Middle Age and Second World War in Europe).
- German Language and Culture.
- Swimming, Italian and International (in particular Indian and German) Cooking.

## Publications

Pre 2000

**1. Proton Transfer in ground and excited electronic states of 2,2'-bipyridil-3,3'-diol: a semiempirical study**

Vincenzo Barone, **Giuseppe Milano**, Laura Orlandini and Carlo Adamo  
*J.Chem Soc. Perkin Trans 2*, 1141, (1995).

**2. A Preliminary study of host-guest interactions in Polymeric Clathrates. An ab-initio Study of the model Complexes Benzene/X<sub>2</sub> (X=F,Cl,Br,I)**

**Giuseppe Milano**, Gaetano Guerra and Luigi Cavallo  
*Eur. J. Inorg. Chem.* 1513, (1998).

**3. Chemical separation by nonoporous crystalline samples of syndiotactic polystyrene**

Gaetano Guerra, **Giuseppe Milano**, Vincenzo Venditto, Fausta Loffredo, OddaRuiz de Ballesteros, Luigi Cavallo and Claudio De Rosa  
*Macromolecular Symposia* 138, 131, (1999).

2000

**4. Thermoplastic Molecular Sieves**

Gaetano Guerra, **Giuseppe Milano**, Vincenzo Venditto, Pellegrino Musto, Luigi Cavallo, Claudio De Rosa  
*Chemistry of Materials* 12, 363, (2000).

**5. Mechanism of Unlike Stereoselectivity in 1-Alkene Primary Insertions: Syndiospecific Propene Polymerization by Brookhart-Type Nickel(II) Catalysts**

**Giuseppe Milano**, Gaetano Guerra, Claudio Pellecchia, Luigi Cavallo  
*Organometallics* 19, 1343, (2000).

**6. Mechanism of Unlike Stereoselectivity in 1-Alkene Primary Insertions: Syndiospecific Propene Polymerization by Brookhart-Type Nickel(II) Catalysts**

**Giuseppe Milano**, Gaetano Guerra, Claudio Pellecchia, Luigi Cavallo  
*Polymer Preprints* (Am. Chem. Soc., Div. Polym. Chem.) 41(1), 454 (2000).

2001

**7. Ab initio and Molecular Mechanics Study of Conformational Selectivity of Chlorinated Compounds Adsorbed in the Clathrate Phase of Syndiotactic Polystyrene. The Role of Electrostatic Host-Guest Interactions.**

**Giuseppe Milano**, Gaetano Guerra, Luigi Cavallo  
*Macromolecular Theory and Simulations* 10, 349, (2001).

**8. Shape and Volume of Cavities in Thermoplastic Molecular Sieves based on Syndiotactic Polystyrene**

**Giuseppe Milano**, Gaetano Guerra, Vincenzo Venditto, Luigi Cavallo, Paolo Ciambelli, Diana Sannino.  
*Chemistry of Materials.* 13, 1506, (2001).

**9. Stereoselectivity and Chemoselectivity in Ziegler-Natta Polymerizations of Conjugated Dienes. 1. Monomers with low energy s-cis  $\eta^1$  coordination**

Chiara Costabile, **Giuseppe Milano**, Luigi Cavallo, Gaetano Guerra  
*Macromolecules*, 34, 7952, (2001).

2002

**10. A Possible Unified Mechanism of like and unlike chain-end stereocontrol for primary propene coordinated polymerizations**

**Giuseppe Milano**, Giuseppe Fiorello, Gaetano Guerra, Luigi Cavallo  
*Macromol. Chem. and Phys.* 203, 1564, (2002).

**11. Stereochemical pseudo-hexad <sup>13</sup>C NMR resonances and regioregular propylene/ethylene copolymers**

Irene Sessa, Dino Romano Ferro, Fabia Grisi, Dario Liguori, **Giuseppe Milano**, Adolfo Zambelli.  
*Macromolecular Chemistry and Physics* 203, 2604, (2002).

**12. Site Chirality as a Messenger in Chain-End Stereocontrolled Propene Polymerization.**

**Giuseppe Milano**, Luigi Cavallo, Gaetano Guerra.  
*Journal of the American Chemical Society* 124, 13368, (2002).

**13. Crystalline orientation and molecular transport properties in nanoporous syndiotactic polystyrene films**

Paola Rizzo; Alexandra R. Albuña, **Giuseppe Milano**,; Vincenzo Venditto, Gaetano Guerra, Giuseppe Mensitieri; Luciano Di Maio.  
*Macromolecular Symposia* 85, 65, (2002).

**14. Mechanism of syndiospecific polymerization of propene promoted by Bis(phenoxyimine) titanium catalysts**

Marina Lamberti, **Giuseppe Milano**, Luigi Cavallo, Gaetano Guerra, Claudio Pellecchia  
*Polymeric Materials Science and Engineering* 87, 44, (2002).

**15. Anisotropic Diffusion of Small Penetrants in the delta Crystalline Phase of Syndiotactic Polystyrene: A Molecular Dynamics Simulation Study**

**Giuseppe Milano**, Gaetano Guerra, Florian Müller-Plathe  
*Chemistry of Materials* 14, 2977, (2002).

**16. Stereoselective Cyclopropanation by Cyclocopolymerization of Butadiene**

Stefania Pragliola, **Giuseppe Milano**, Gaetano Guerra, Pasquale Longo,  
*Journal of the American Chemical Society* 124, 3502, (2002).

2003

**17. E Stereoregular 1,1 and 1,3 Constitutional Units from 1,3-Butadiene in Copolymerizations Catalyzed by a Highly Hindered C<sub>2</sub> Symmetric Metallocene**

Pasquale Longo, Stefania Pragliola, **Giuseppe Milano**, Gaetano Guerra  
*Journal of the American Chemical Society* 125, 4799, (2003).

**18. Butadiene insertion and Constitutional Units in Ethene Copolymerizations by C<sub>2</sub>-Symmetric Metallocenes**

Pasquale Longo, Mariagrazia Napoli, Stefania Pragliola, Chiara Costabile, **Giuseppe Milano**, Gaetano Guerra.  
*Macromolecules* 36, 9067, (2003).

**19. Chlorinated Guest Orientation and Mobility in Chlathrate Structures Formed with Syndiotactic Polystyrene**

Alexandra R. Albuña, Sergio Di Masi, Paola Rizzo, **Giuseppe Milano**, Pellegrino Musto, Gaetano Guerra.  
*Macromolecules* 36, 8695, (2003).

2004

**20. Stereoselectivity and Chemoselectivity in Ziegler-Natta Polymerizations of Conjugated Dienes. 2. Mechanism for 1,2 syndiotactic polymerization of diene monomers with high energy s-cis  $\eta^4$  coordination**

Chiara Costabile, **Giuseppe Milano**, Luigi Cavallo, Pasquale Longo, Gaetano Guerra, Adolfo Zambelli.

*Polymer* 45, 467, (2004).

**21. Cyclohexane-Benzene Mixtures: Thermodynamics and Structure from Atomistic Simulations**

**Giuseppe Milano**, Florian Müller-Plathe

*J. Phys. Chem. B* 108, 7415, (2004).

**22. Statistical Physics of Polymers An Introduction. Kawakatsu, Toshihiro.**

**Giuseppe Milano**

*Soft Materials* 2, 215, (2004).

2005

**23. (E)-(Z) Selectivity in the Polymerization of 2-Butene Promoted by Ni(II) Brookhart-Type Catalysts**

**Giuseppe Milano**, Gaetano Guerra, Mina Mazzeo, Claudio Pellecchia, Luigi Cavallo

*Macromolecules* 38, 2072, (2005).

**24. Multicentred Gaussian-Based Potentials for Coarse-Grained Polymer Simulations: Linking Atomistic and Mesoscopic Scales**

**Giuseppe Milano**, Sylvain Goudeau, Florian Müller-Plathe

*J. Polymer. Science Part B: Polymer Physics* 43, 871, (2005).

**25. Orientation and Microenvironment of Naftalene Guest in the Host Nanoporous Phase of Syndiotactic Polystyrene**

Vincenzo Venditto, **Giuseppe Milano**, Anna De Girolamo del Mauro, Gaetano Guerra, Jun Mochizuchi, Hideyuchi Itagaky

*Macromolecules* 38, 3696, (2005).

**26. Host-Guest Interactions, Guest Dynamics and Morphology in Syndiotactic Polystyrene Nanoporous and Clathrate Crystalline Phases in "Structure and Dynamics in Macromolecular Systems with Specific Interactions"**

Gaetano Guerra, Alexandra Alburnia, Christophe Daniel, **Giuseppe Milano**, Paola Rizzo, Vincenzo Venditto

pp 91-100 Ed. K. Adachi, T. Sato Osaka University Press, Osaka 2005.

**27. Thermoplastic Molecular Sieves: New Polymeric Materials for Molecular Packaging in "New Polymeric Materials"**

**Giuseppe Milano**, Christophe Daniel, Vincenzo Venditto, Paola Rizzo, Gaetano Guerra, Pellegrino Musto, Giuseppe Mensitieri.

Chap. 13, p 171 Edited by L. S. Korugic-Karasz, W. J. MacKnight, E. Martuscelli ACS Books, Washington DC, 2005.

**28. Mapping Atomistic Simulations to Mesoscopic Models: A Systematic Coarse-Graining Procedure for Vinyl Polymer Chains**

Giuseppe Milano, Florian Müller-Plathe  
*J. Phys. Chem. B* 109; 18609, (2005).

**29. A clear Cut Experimental Method to Discriminate between In-Plane and Out-of-Plane Molecular Transition Moments**

Alexandra R. Alburnia, Giuseppe Milano, Vincenzo Venditto, Gaetano Guerra  
*J. Am. Chem. Soc.* 127, 13114, (2005).

2006

**30. Anisotropic Guest Diffusion in the Crystalline Host Phase of Syndiotactic Polystyrene: Transport Kinetics in Films with Three Different Uniplanar Orientation of the Host Phase**

Vincenzo Venditto, Anna de Girolamo del Mauro, Giuseppe Mensitieri, Giuseppe Milano, Pellegrino Musto, Paola Rizzo, Gaetano Guerra  
*Chemistry of Materials* 18, 2205, (2006).

**31. Synthetic Polymers and Biomembranes. How do they interact?: Atomistic Molecular Dynamics Simulation Study of PEO in contact with a DMPC Lipid Bilayer**

Sandeep Pal, Giuseppe Milano, Danilo Roccatano  
*J. Phys. Chem. B* 110; 26170, (2006).

**32. Dynamics of benzene guest inside a self-assembled cylindrical capsule: A combined solid-state H-2 NMR and molecular dynamics simulation study**

Alexandra R. Alburnia, Carmine Gaeta, Placido Neri, Alfonso Grassi, Giuseppe Milano  
*J. Phys. Chem. B* 110; 19207, (2006).

**33. Oriented nanoporous host delta phases of syndiotactic polystyrene as a tool for spectroscopic investigation of guest molecules**

Alexandra R. Alburnia, Alfonso Grassi, Giuseppe Milano, Paola Rizzo, Vincenzo Venditto, Pellegrino Musto, Gaetano Guerra  
*Macromolecular Symposia* 234,102, (2006).

2007

**34. From mesoscale back to atomistic models: A fast reverse-mapping procedure for vinyl polymer chains**

Giuseppe Santangelo, Andrea Di Matteo, Florian Müller-Plathe, Giuseppe Milano  
*J. Phys. Chem. B* 111; 2765, (2007).

**35. Coarse-grained and reverse-mapped united-atom simulations of long-chain atactic polystyrene melts: Structure, thermodynamic properties, chain conformation, and entanglements**

Theodora Spyriouni, Christos Tzoumanekas, Doros Theodorou, Florian Müller-Plathe, Giuseppe Milano  
*Macromolecules* 40, 3876, (2007).

**36. Viscosity and Structural Alteration of a Coarse-Grained Model of Polystyrene under Steady Shear Flow Studied by Reverse Nonequilibrium Molecular Dynamics**

Xiaoyu Chen, Paola Carbone, Welch L. Cavalcanti, Giuseppe Milano, Florian Müller-Plathe  
*Macromolecules* 40, 8087, (2007).



**37. Understanding at molecular level of nanoporous and co-crystalline materials based on syndiotactic polystyrene**

Giuseppe Milano, Gaetano Guerra  
PROGRESS IN MATERIALS SCIENCE 54, 68, (2009)

**38. Backmapping coarse-grained polymer models under sheared nonequilibrium conditions**

Xiaoyu Chen, Paola Carbone, Giuseppe Santangelo, Andrea Di Matteo, Giuseppe Milano and Florian Müller-Plathe  
*Phys. Chem. Chem. Phys.*, (2009), DOI: 10.1039/b817895j

**39. A molecular model for H<sub>2</sub> interactions in aliphatic and aromatic hydrocarbons**

Susana Figueroa-Gerstenmaier, Simona Giudice, Luigi Cavallo, and Giuseppe Milano  
*Phys. Chem. Chem. Phys.* In Press

**40. Reactivity of a cationic alkyl amino-functionalized cyclopentadienyl aluminum compound with olefins: NMR observation and computational investigation of the single propene insertion product into an Al-C bond**

Daniela Pappalardo, Massimiliano Mella, Giuseppe Milano, Claudio Pellecchia  
*Organometallics* In Press

**41. Hybrid Particle-Field Molecular Dynamics Simulations for Dense Polymer Systems**

Giuseppe Milano, Toshihiro Kawakatsu  
*Manuscript in Preparation for J. Chem. Phys.*

**42. Polystyrene/Gold Nanoparticle Interfaces: All atom Structures from Multiscale Molecular Dynamics Simulations**

Giuseppe Milano, Giuseppe Santangelo, Francesco Ragone, Luigi Cavallo, Andrea Di Matteo  
*Manuscript in Preparation*

**43. A Charge Transfer Metropolis Monte Carlo Algorithm for Automatic Point Charges Parametrization:**

Andrea Correa, Luigi Cavallo, Giuseppe Milano  
In Preparation for Journal of Computational Chemistry

Selected Conference Communications and invited Talks

**1. Models for syndiospecific chain-end controlled propene polymerisation with Brookhart-type Ni(II) catalysts**

G. Milano, G. Guerra and L. Cavallo  
Poster: "Workshop on advances in organometallics and olefin polymerisation." (Ferrara 28-29 Maggio 1998)

**2. Chemical separation by nanoporous crystalline samples of syndiotactic polystyrene**

G. Guerra, G. Milano, V. Venditto, F. Loffredo, O. Ruiz de Ballesteros, L. Cavallo and C. De Rosa  
Coauthor of Oral: "2nd International Conference on Polymer-Solvent Complexes and Intercalates" dal titolo (Ischia 31-Agosto 4-Settembre 1998)

**3. Sorption of Chlorinated Solvents and their Mixtures in Semicrystalline Syndiotactic Polystyrene: Role of Adsorption in the Crystalline Phase**

Giuseppe Mensitieri, Gaetano Guerra, Giuseppe Milano, Pellegrino Musto, Vincenzo Venditto  
Coauthor of Oral: Annual Conference of AIChE (American Institute of Chemical Engineers) fourth topical conference on separation science and technology Dallas 31 October –1 November 1999

**4. Mechanism of Unlike Stereoselectivity in 1-Alkene Primary Insertions: Syndiospecific Propene Polymerization by Brookhart-Type Nickel(II) Catalysts**

Giuseppe Milano, Gaetano Guerra, Claudio Pellecchia, Luigi Cavallo.  
Poster: 219th ACS National Meeting, San Francisco, CA, 26-30 March 2000.

**5. Mechanisms of chain-end stereoselectivity in propene polymerizations**

Giuseppe Milano, Giuseppe Fiorello Gaetano Guerra, Luigi Cavallo.  
Poster: OCOP2000 Organometallic Catalysts and Olefin Polymerization (New Millennium International Conference). Oslo 18-22 June 2000.

**6. Density functional studies of mechanism of Ziegler-Natta dienes polymerizations**

Chiara Costabile, Giuseppe Milano, Gaetano Guerra, Luigi Cavallo.  
Poster: OCOP2000 Organometallic Catalysts and Olefin Polymerization (New Millennium International Conference). Oslo 18-22 June 2000.

**7. Thermoplastic Molecular Sieves based on Syndiotactic Polystyrene**

Gaetano Guerra, Fausta Loffredo, Giuseppe Milano, Vincenzo Venditto, Pellegrino Musto, Giuseppe Mensitieri.  
Coauthor of Oral: World Polymer Congress IUPAC Macro 2000 (38th Macromolecular IUPAC Symposium) Warsaw, Poland, 9-14<sup>th</sup> July 2000.

**8. Mechanisms of chain-end stereoselectivity in propene primary insertions**

G. Milano, G. Fiorello, G. Guerra, L. Cavallo  
Oral: 3rd Workshop on 'Advances on Insertion Polymerisation'  
Ischia, 11-13 September 2000

**9. Mechanisms of chain-end stereoselectivity in propene secondary insertions**

G. Milano, G. Fiorello, G. Guerra, L. Cavallo  
Poster: 3rd Workshop on 'Advances on Insertion Polymerisation'  
Ischia, 11-13 September 2000

**10. Density functional studies of mechanisms of Ziegler-Natta dienes polymerizations**

Coauthor of Oral: C. Costabile, G. Milano, G. Guerra, Luigi Cavallo  
3rd Workshop on 'Advances on Insertion Polymerisation'  
Ischia, 11-13 September 2000

**11. Thermoplastic Molecular Sieves Based on Syndiotactic Polystyrene**

Coauthor of Oral: G. Guerra, G. Milano, V. Venditto, F. Loffredo, P. Musto, G. Mensitieri  
EPF-Europolymer Congress June 2001. Eindhoven, Plenary Lecture 20.

**12. Transport Properties of Small Molecules in the delta Crystalline Phase of Syndiotactic Polystyrene: Simulations and Experiments**

G. Milano, G. Guerra, F. Müller-Plathe  
Oral: Molecular Modelling on Membrane Research 2002 GKSS in Teltow (Germany), 22-24 May 2002

**13. (E)-(Z) Selectivity in the Polymerization of 2-Butene Promoted by Ni(II) Brookhart-Type Catalysts**

Oral: European Polymer Conference on Stereospecific Polymerization and Stereoregular Polymers – EUPOC 2003 Milano 8 - 12 June 2003

**14. Flory-Huggins Parameter from Atomistic Molecular Dynamics Simulations  
Giuseppe Milano**

Poster: "NIC Winter School Computational Soft Matter: From Synthetic Polymers to Proteins"  
Winter School, 29 Feb. - 6 March 2004 Gustav-Stresemann-Institut, Bonn.

**15. Computational Chemistry and Experiments**

Giuseppe Milano

Invited Talk: Max-Planck-Institut für Eisenforschung invited by Prof. Martin Stratman.  
Duesseldorf 29 January 2004.

**16. Bridging the Scales: Coarse-Grained Simulations of Polymeric Materials**

Giuseppe Milano

Invited Talk: Zürich ETH Laboratorium für Physicalische Chemie, invited by Prof. Wilfred van Gunsteren 24<sup>th</sup>  
August 2005

**17. YAMMT: Yet another Multiscale Modeling Talk Giuseppe Milano**

Giuseppe Milano

Invited Talk: Technische Universität of Darmstadt, Theoretische Physikalische Chemie Group, invited by Prof.  
Florian Müller-Plathe 13<sup>th</sup> September 2005

**18. Multiscale Modelling and Nanofabrication**

Giuseppe Milano

Invited Talk: WorkshopNanoMetrology 2007 Metrology for Nanotechnology  
June 14-15, 2007 National Institute of Metrological Research – INRIM Torino - Italy

**19. Multiscale Modelling in Polymer Science: from atomistic to mesoscale simulations**

Oral: Mesoscale Modeling for Complex Fluids and Flows, Department of Physics University of Oxford 25-27  
June 2007.

**20. Model the Nanoscale with Chemical Accuracy. How Multiscale Modelling Simulations Can Help.**

Invited Talk: Tohoku University, Sendai, Department of Physics, Theoretical Condensed Matter and  
Statistical Physics Group, Sendai 12 September 2007.

**21. Possible Multiscale Approaches for Nanocomposites Materials in Aeronautics**

Invited Talk: Opening talk at First Meeting of the Multiscale Modeling Working Group

(Mind Sh@re Community Corporate Project of Finmeccanica)

Alenia Aeronautica January 30<sup>th</sup> 2009 Pomigliano

See: <http://www.alenia-aeronautica.it/eng/Pages/Home.aspx>