# MATTEO MAESTRI

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**Last update: April 2018**

## EDUCATION

Politecnico di Milano, Italy, 2008
Ph. D. *summa cum laude* in Chemical Engineering and Industrial Chemistry

Politecnico di Milano, Italy, 2004
Laurea (Master of Science) *summa cum laude* in Chemical Engineering

## RESEARCH EXPERIENCE

Associate Professor
Politecnico di Milano, Italy, 2015 – present

Assistant Professor
Politecnico di Milano, Italy, 2008 – 2015

Professorship Habilitation (Abilitazione Scientifica Nazionale), 2013

Alexander von Humboldt Fellow
Department of Chemistry, Catalysis Research Center,
Technische Universität München (Garching, Germany), 2011

Alexander von Humboldt Fellow
Fritz-Haber-Institut der Max-Planck-Gesellschaft (Berlin, Germany), 2009 – 2010

Contract Researcher/Lecturer
Politecnico di Milano, Italy, 2007 – 2008

Visiting Scholar (Advisor: Prof. D.G. Vlachos)
Department of Chemical Engineering, Center for Catalytic Science and Technology
University of Delaware (USA), 2006 – 2007

## THESIS AND POSTDOCTORAL SUPERVISORS

Prof. Enrico Tronconi, Politecnico di Milano, Italy – Ph. D. thesis supervisor

Prof. Karsten Reuter, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany (now at Technische Universität München, Germany), postdoctoral supervisor

## HONORS/AWARDS

- 2018: Pregl Lecture, Kemijski inštitut, National Institute of Chemistry – Ljubljana, Slovenia
- 2017: Listed in the selection of Italy's 100 best under-40 researchers currently active both in Italy and abroad, CARTADITALIA - Istituto Italiano di Cultura, Brussels
- 2016: ERC Starting Grant - ERC, European Research Council (**success rate: 10%)**
- 2016. Selected for Early Career Series paper in ChemPlusChem (Wiley)
- 2015: SIR (Scientific Independence of Young Researchers) - MIUR, Rome (**success rate: 3%**)
- 2014: appointed as a *member of the International Scientific Committee* of ISCRE 24 (International Symposium of Chemical Reaction Engineering) to be held in Minneapolis, USA, June 12-15, 2016
- 2012: *Young Scientist Award* at the 15th International Congress on Catalysis (Munich, Germany, July 1-6, 2012), presented by the International Association of Catalysis Societies (IACS).
- 2012: *Alexander von Humboldt* grant for financial assistance at the 15th International Congress on catalysis (Munich, Germany, July 1-6, 2012)
- 2011: Cover picture *Angewandte Chemie Int. Ed*. (vol. 50 – Issue 17)
- 2010: *Young Researcher Award* at the 21st International Symposium on Chemical Reaction Engineer (ISCRE), June 13-16, 2010, Philadelphia, USA
- 2010: mentioned in Chem. Eur. J. 16 (2010) 13888-13893 for participation to EYCA 2010
- 2009: *Alexander von Humboldt Research Fellowship* **(success rate 25%)**
- 2008: *Young Scientist Award* at the 14th International Congress on Catalysis (Seoul, Korea, July 13-18, 2008), presented by the International Association of Catalysis Societies (IACS).

## RESEARCH INTERESTS

During his research activity, he has developed interdisciplinary and multiscale skills and expertise, spanning from macroscopic **chemical reaction engineering** to **first-principles studies addressing elementary processes at the nanoscale**. This research experience was gained in an interdisciplinary corridor between catalysis and reaction engineering and between physical chemistry (semi-empirical and first-principles methods) and chemical engineering (transport phenomena, applied mathematics, numerical analysis) in close interaction with kinetic and spectroscopic experiments.

His main research interests are:

i. Heterogeneous catalysis.
ii. Chemical and catalytic reactor engineering.
iii. First principles multiscale modeling of catalytic chemical processes.
iv. Microkinetic modeling and analysis.
v. Process analysis and intensification.
vi. Computational fluid dynamics of reacting flows.
vii. Electronic structure calculations of materials.
viii. DFT calculations of reaction pathways.
ix. Kinetic-Monte-Carlo simulations.

**GRANTS in the last 3 years**

Matteo Maestri is **principal investigator** of research projects for a total budget in excess of 2,000,000 Euro and in excess of 25 Mio cpu-hours at international supercomputing centres.

*Peer-reviewed research projects*:

- ***ERC, European Research Council*** - call: ERC-Starting Grant -2015 - project: SHAPE - STRUCTURE-DEPENDENT MICROKINETIC MODELING OF HETEROGENEOUS CATALYTIC PROCESSES - from May 2016 to April 2021 - Grant**: 1,496,250 Euro** (success rate: 10%)
- ***MIUR, Ministero della istruzione, della ricerca e dell'università, Italy***, call FARE (Framework per l'attrazione e il rafforzamento delle eccellenze per la ricerca in Italia) – project: SPOON - SURFACE PLASMON RESONANCE FOR THE IN-OPERANDO CHARACTERIZATION OF SHAPE AND SIZE OF SUPPORTED METALLIC NANOPARTICLES – from January 2018 to January 2022 – Grant: **151,000 Euro**
- ***MIUR, Ministero della istruzione, della ricerca e dell'università, Italy*** – call: SIR (Scientific Independence of Young Researchers) 2014 – project: THEOREMA -INTEGRATED THEORETICAL-EXPERIMENTAL METHODOLOGY FOR OPERANDO-RAMAN KINETIC STUDIES IN HETEROGENEOUS CATALYSIS – from October 2015 to October 2018 - Grant: **385,000 Euro** (success rate 3%)
- ***CINECA Supercomputing Centre (Bologna, Italy)*** – project: PROSPECT - ASSESSMENT OF CATALYST DESCRIPTORS FOR THE CO2 ACTIVATION ON LOW INDEX METALLIC SURFACES – from July 2016 to June 2017 (ISCRA CALL 2016) – Grant: **3 Million CPU hours**
- ***CINECA Supercomputing Centre (Bologna, Italy)*** – project: 1pNOx - FIRST-PRINCIPLES ASSESSMENT OF THE METAL EFFECT IN NOx CATALYTIC REDUCTION PROCESSES – from July 2016 to June 2017 (LISA CALL 2016) – Grant: **3 Million CPU hours**
- ***CINECA Supercomputing Centre (Bologna, Italy)*** – project: CON CAT - FIRST PRINCIPLES ASSESSMENT OF CATALYSIS BY CONFINEMENT IN MICROPOROUS SILICEOUS ZEOLITES – from June 2014 to June 2015 (ISCRA CALL 2014) – Grant: **7 Million CPU hours**
- ***CINECA Supercomputing Centre (Bologna, Italy)*** – project: FBI – FIRST PRINCIPLES ASSESSMENT OF UBI-METHOD FOR HIERARCHICAL MICROKINETIC MODELING OF COMPLEX CATALYTIC PROCESSES – from June 2014 to June 2015 (LISA CALL 2014) – Grant: **3.5 Million CPU hours**
- ***CINECA Supercomputing Centre (Bologna, Italy)*** – project: CREAM - ADVANCED MICROREACTOR MODELING FOR ENERGY AND ENVIRONMENT – from November 2013 to November 2014 (LISA CALL 2013) – Grant: **3 Million CPU hours**
- ***Leibniz Supercomputing Centre (Munich, Germany)*** - project: pr47ma: HYDROGEN PRODUCTION AT THE MICROSCALE: THEORETICAL ASSESSMENT OF THE SURFACE REACTIVITY of MILLISECOND-CONTACT-TIME REFORMERS (extended on the basis of peer-review evaluation of results obtained in the first 2 years) - from May 2010 to May 2016 – Grant: **12 Million CPU hours**

*Industrial research projects*:

He has been also Principal Investigator for research funding from industry in excess of **300,000 Euro** in the last 3 years.

## SCIENTIFIC SERVICES

*Co-organized workshops and conferences*:

1. *DeMiR 2011: From Detailed Microkinetics to the Reactor*, European Workshop on Multiscale Catalytic Reactor Engineering, TUM, Munich, Sept. 6, 2011, organized by **M. Maestri**, R. Horn and K. Reuter
2. *Colloquium on Chemical Reaction Engineering 2013* – sponsored by the European Federation of Chemical Engineering (EFCE): "First-principles methods in Chemical Reaction Engineering", organized by G. Groppi, **M. Maestri**, E. Tronconi, Politecnico di Milano, Italy, October 17-18, 2013
3. member *of the International Scientific Committee* of ISCRE 24 (International Symposium of Chemical Reaction Engineering) Minneapolis, USA, June 12-15, 2016
4. organizer (together with prof. J. Thybaut, Gent University) of the International workshop "Bridging Laboratory Chemical Kinetics to Industrial Scale Reactors", Firenze, August 23-25, 2017
5. member of the *organizing committee* of ISCRE 25 (International Symposium of Chemical Reaction Engineering) to be held in Firenze, Italy, May 2018
6. organizer (together with prof. J. Thybaut, Gent University) of the International workshop "Bridging Laboratory Chemical Kinetics to Industrial Scale Reactors – 2nd edition", Firenze, May 23-27, 2018

*Reviewer for the following scientific journals*: Journal of Catalysis, ACS Catalysis, Angewandte Chemie, Applied Catalysis A: General, Applied Catalysis B: Environmental, Catalysis Today, Chemical Engineering Journal, Chemical Engineering Science, Industrial and Engineering Chemistry Research, International Journal of Chemical Kinetics, International Journal of Hydrogen Energy, Computers and Chemical Engineering, ChemCatChem, ChemSusChem, Proceedings of Combustion Institute, Reaction Chemistry and Engineering

*Reviewer for the following research foundations*: DFG (Deutsche Forschungsgemeinschaft, German Research Foundation), FWO (Fonds Wetenschappelijk Onderzoek - Vlaanderen, Belgium), KAUST -Competitive Research Grant Scheme (CRG), National Science Centre, Poland, NWO (Netherlands Organisation for Scientific Research)

## ACTIVE SCIENTIFIC COLLABORATIONS

"*Numerical methods for the computational fluid dynamics of catalytic reactors*"
Prof. Anthony G. Dixon – Worcester Polytechnic Institute, Worcester, MA, USA

"*First-principles assessment of catalysis by confinement in microporous siliceous zeolites*"
Prof. Enrique Iglesia – University of California, Berkeley, CA, USA

"*First principles assessment of $CO_2$ activation pathways on metal catalysts*"
Dr. Simone Piccinin – SISSA, Trieste, Italy

"*Development of models for the prediction of the crystal habit in reacting conditions*"
Prof. Aloysius Soon – Yonsei University, Seoul, South Korea

"*Coupling kinetic Monte Carlo simulations with CFD in heterogeneous catalysis*"
Prof. Michail Stamatakis – University College London, London, UK

"*Advanced optimization of catalytic reactors using microkinetic modeling*"
Prof. Kai Sundmacher – Max-Planck-Institut, Magdeburg, Germany

## TEACHING ACTIVITY

Professor of *Advanced Catalytic Reactor Design*, Politecnico di Milano, 2011 – present
Graduate, Chemical Engineering, Politecnico di Milano

Professor of *Petroleoum Technologies and Biofuels*, Politecnico di Milano, 2016 – present
Graduate, Energy Engineering, Politecnico di Milano

## RESEARCH PUBLICATIONS

### Highlights and highly cited papers (numbers refer to papers below):

i. P8 in *Journal of Catalysis* was included in the Top25 hottest articles list (most downloaded) of Journal of Catalysis for the period October-December 2008

ii. P9 in *A.I.Ch.E. Journal* was included in the 2009 Top10 most cited articles list of A.I.Ch.E. Journal

iii. P10 in *A.I.Ch.E. Journal* was included in the 2009 Top10 most cited articles list of A.I.Ch.E. Journal

iv. P14 in *Angewandte Chemie Int. Ed.* was mentioned in the Psi-k News Letter "Ab initio calculation of complex processes in materials" n. 104 April 2011

v. P15 in *Angewandte Chemie Int. Ed.* was classified VIP (Very Important Publication)

vi. P15 in *Angewandte Chemie Int. Ed.* was selected for the cover picture of *Angewandte Chemie International Edition (Vol. 50 Issue 17)*

vii. P17 in *Chemical Engineering Science* was mentioned in the Psi-k News Letter "Ab initio calculation of complex processes in materials" n. 110 April 2012

viii. P19 in *Chemical Engineering Science* was included in the Top25 hottest articles list (most downloaded) of Chemical Engineering Science for the period May-July 2013

ix. P23 in *ACS Catalysis* featured in *ACS Editors' Choice*

### Invited papers/book chapters (* = corresponding author):

IP1) **M. Maestri**, E. Tronconi, Characteristics of fixed beds (*invited review on the design of fixed bed reactors*) – EUROKIN – TASK 5C (100 pages), EUROKIN internal document (www.eurokin.org)

IP2) I.Tavazzi, **M. Maestri**, A. Beretta, G. Groppi, P. Forzatti, $H_2$ production for low emission GT via $CH_4$ fuel rich combustion, in *Catalytic Combustion*, Editors: P. Forzatti, F.Groppi, P. Ciambelli, D. Sannino, 1 (2005) 77–82; PoliPress, Milano, Italy. ISBN 88-7398-015-5

IP3) **M. Maestri**, D.G. Vlachos, A. Beretta, P. Forzatti, G. Groppi, E. Tronconi, Microkinetic modeling of heterogenous catalysis: from the rate equation to the rate constant, Chemical Engineering greetings to prof. Eliseo Ranzi in occasion of his 65$^{th}$ birthday, M. Dente Editor, 2008, pp. 295-302, AIDIC, Milano, Italy, ISBN 0390-2358

IP4) A. Donazzi, D. Livio, **M. Maestri**, A. Beretta, G. Groppi, E. Tronconi, P. Forzatti, Interaction of homogeneous and heterogeneous chemistry in short-contact-time catalytic partial oxidation of propane probed by spatially resolved sampling techniques, Chemical Engineering greetings to prof. Sauro Pierucci in occasion of his 65$^{th}$ birthday, M. Dente Editor, 2011, pp. 91-97, AIDIC, Milano, Italy, ISSN 2036-5969

IP5) **M. Maestri***, Microkinetic Analysis of Complex Chemical Processes at Surfaces, *book chapter in "New Strategies in Chemical Synthesis and Catalysis"*, Ed. B. Pignataro, Wiley – VCH Weinheim, 2012, 219–246, ISBN978-3-527-33090-4

IP6) A. Beretta, A. Donazzi, G. Groppi, **M. Maestri**, E. Tronconi and P. Forzatti, Gaining insight into the kinetics of partial oxidation of light hydrocarbons on Rh, through a multiscale methodology based on advanced experimental and modeling techniques, book chapter in *"Catalysis: Volume 25"* Eds. James J Spivey, Yi-Fan Han, K M Dooley, Royal Society of Chemistry, 2013, 25, 1-49, DOI:10.1039/9781849737203-00001, ISBN 978-1-84973-578-0

IP7) S. Rebughini, M. Bracconi, A. Cuoci, **M. Maestri***, "Catalysis Engineering: from the catalytic material to the catalytic reactor", book chapter in "*Operando studies in heterogeneous catalysis*", Edited by I. Groot and J. Frenken (Leiden University, The Netherlands), Springer-Verlag, 114 (2017) 189 - 218

IP8) T. Maffei, S. Rebughini, G. Gentile, S. Lipp, A. Cuoci and **M. Maestri***, CFD Analysis of the Channel Shape Effect in Monolith Catalysts for the CH4 Partial Oxidation on Rh, Chemie Ingenieur Technik, 86 (2014) 1099-1106, special issue edited by M. Nilles (BASF) and G. Wozny (TU- Berlin)

IP9) Z.B. Ding, M. Tommasini, **M. Maestri***, First-principles simulation of Raman spectra of adsorbates on metal surfaces, *ChemPlusChem*, 82 (2017) 924-93 (Early Career Series paper)

**Patents**

B1) A. Beretta, P. Forzatti, G. Groppi, **M. Maestri,** E. Tronconi, Sistema catalitico e suo uso in processi di ossidazione parziale e reforming autotermico, Italian Patent Application MI2010A001480 – Patent owner: Politecnico di Milano – Priority: 3/8/2010

**Scientific Refereed Journal Publications (* = corresponding author)**

P1) **M. Maestri**, A. Beretta, G. Groppi, E. Tronconi, P. Forzatti, Comparison among structured and packed-bed reactors for the catalytic partial oxidation of methane to syngas, *Catalysis Today*, 105 (2005) 709–717.

P2) **M. Maestri**, A. Beretta, G. Groppi, E. Tronconi, P. Forzatti, Modelling of fixed-bed reactors for the catalytic partila oxidation of methane to syngas: a comparison among structured and packed bed reactors, *Chemical Engineering Transactions*, S. Pierucci Editor, 6 (2005), 13–18, AIDIC, Milano, Italy. ISBN 88-900775-7-3.

P3) I. Tavazzi, **M. Maestri**, A. Beretta, G. Groppi, E. Tronconi, P. Forzatti, Steady state and transient analysis of a $CH_4$ catalytic partial oxidation reformer, *A.I.Ch.E. Journal*, 52 (2006) 3234–3245.

P4) I. Tavazzi, A. Beretta, G. Groppi, **M. Maestri**, E. Tronconi, P. Forzatti, Experimental and modeling analysis of the effect of catalyst aging on the performance of a short contact time adiabatic $CH_4$-CPO reactor, *Catalysis Today*, 129 (2007) 372–379.

P5) I. Tavazzi, A. Beretta, G. Groppi, A. Donazzi, **M. Maestri**, E. Tronconi, P. Forzatti, Catalytic partial oxidation of $CH_4$ and $C_3H_8$: experimental and modeling study of the dynamic and steady state behavior of a pilot-scale reformer, in *Studies in Surface Science and Catalysis*, 67 (2007) 319–324.

P6) **M. Maestri**, A. Beretta, G. Groppi, T. Faravelli, E. Tronconi, Role of gas-phase chemistry in the rich combustion of $H_2$ and CO over a $Rh/Al_2O_3$ catalyst in annular reactor, *Chemical Engineering Science*, 62 (2007) 4992–4997.

P7) **M. Maestri**, A. Beretta, G. Groppi, T. Faravelli, E. Tronconi, D.G. Vlachos, Two-dimensional detailed modeling of $H_2$ fuel rich combustion over $Rh/Al_2O_3$ catalyst, *Chemical Engineering Science*, 63 (2008) 2657-2669.

P8) **M. Maestri**, D.G. Vlachos, A. Beretta, G. Groppi, E. Tronconi, Steam and Dry Reforming of Methane on Rh: microkinetic analysis and hierarchy of kinetic models, *Journal of Catalysis*, 259 (2008) 211-222 (This paper was included in the *Top25 hottest articles list* (most downloaded) of *Journal of Catalysis* for the period October-December 2008).

P9) G.D. Stefanidis, D.G. Vlachos, N.K. Kaisare, **M. Maestri**, Methane steam reforming at microscale: Operation strategies for variable power output at millisecond contact times, *A.I.Ch.E. Journal*, 55 (2009) 180-191 (This paper was included in the *2009 Top10 most cited articles list* of *A.I.Ch.E. Journal*).

P10) **M. Maestri**, D.G. Vlachos, A. Beretta, G. Groppi, E. Tronconi, A $C_1$ microkinetic model for the $CH_4$ conversion to syngas on Rh, *A.I.Ch.E. Journal*, 55 (2009) 993 – 1008. (This paper was included in the *2009 Top10 most cited articles list* of *A.I.Ch.E. Journal*).

P11) **M. Maestri**, D.G. Vlachos, A. Beretta, P. Forzatti, G. Groppi, E. Tronconi, Dominant reaction pathways in the catalytic partial oxidation of methane on Rh, *Topics in Catalysis*, 52 (2009) 1983 – 1988

P12) A. Donazzi, **M. Maestri**, B.C. Micheal, A. Beretta, P. Forzatti, G. Groppi, E. Tronconi, L.D. Schmidt, D.G. Vlachos, Microkinetic modeling of spatially resolved autothermal $CH_4$ CPO experiments over Rh-coated foams, *Journal of Catalysis*, 275 (2010) 270 – 279

P13) A. Donazzi, **M. Maestri**, A. Beretta, G. Groppi, E. Tronconi, P. Forzatti, Microkinetic analysis of $CH_4$-CPO tests with $CO_2$-diluted feed streams, *Applied Catalysis A: General*, 391 (2011) 350 – 359

P14) **M. Maestri***, K. Reuter, Semi-empirical rate constants for complex chemical kinetics: first principles assessment and rational refinement, *Angewandte Chemie Int. Ed*., 50 (2011) 1194 – 1197

P15) A. Donazzi, D. Livio, **M. Maestri**, A. Beretta, G. Groppi, E. Tronconi, P. Forzatti, Synergy of homogenous and heterogeneous chemistry probed by in-situ spatially resolved measurements of temperature and composition, *Angewandte Chemie Int. Ed.*, 50 (2011) 3943 - 3946 **(VIP publication + cover picture**)

P16) A. Beretta, A. Donazzi, D. Livio, **M. Maestri**, G. Groppi, E. Tronconi, P. Forzatti, Optimal design of a $CH_4$ CPO-reformer with honeycomb catalyst: combined effect of catalyst load and channel size, *Catalysis Today*, 171 (2011) 79 – 83

P17) **M. Maestri***, K. Reuter, Molecular-level understanding of WGS and reverse WGS reactions on Rh through hierarchical multiscale approach, *Chemical Engineering Science*, 74 (2012) 296-299

P18) D. Pagani, D. Livio, A. Donazzi, A. Beretta, G. Groppi, **M. Maestri**, E. Tronconi, A kinetic analysis of the partial oxidation of propane over a 2% $Rh/Al_2O_3$ catalyst in annular microreactor, Catalysis Today, 197 (2012) 266-280

P19) **M. Maestri*** and A. Cuoci, Coupling CFD with detailed microkinetic modeling in heterogeneous catalysis, *Chemical Engineering Science*, 96 (2013) 106-117 (This paper was included in the *Top25 hottest articles list* (most downloaded) of Chemical Engineering Science for the period May-July 2013).

P20) D. Pagani, D. Livio, A. Donazzi, **M. Maestri**, A. Beretta, G. Groppi, and P. Forzatti, A kinetic investigation of the Catalytic Partial Oxidation of propylene over a $Rh/Al_2O_3$ catalyst, *Industrial and Engineering Chemistry Research*, 53 (2014) 1804–1815

P21) **M. Maestri***, D. Livio, A. Beretta, G. Groppi, Hierarchical refinement of complex microkinetic models: assessment of the role of WGS and r-WGS pathways in $CH_4$ Partial Oxidation on Rh, *Industrial and Engineering Chemistry Research*, 53 (2014) 10914-10928

P22) T. Maffei, S. Rebughini, G. Gentile, S. Lipp, A. Cuoci and **M. Maestri***, CFD Analysis of the Channel Shape Effect in Monolith Catalysts for the CH4 Partial Oxidation on Rh, *Chemie Ingenieur Technik*, 86 (2014) 1099-1106 (invited)

P23) S. Matera, **M. Maestri***, A. Cuoci, K. Reuter, Coupling kinetic Monte Carlo simluations and CFD in heterogeneous catalysis, *ACS Catalysis*, 4 (2014) 4081–4092

P24) F. Karst, H.J. Freund, **M. Maestri**, K. Sundmacher, Multiscale Chemical Process Design Exemplified for a PEM Fuel Cell Process, *Chemie Ingenieur Technik*, 86 (2014) 2075–2088

P25) L. Dietz, S. Piccinin, **M. Maestri***, First-principles assessment of $CO_2$ activation pathways over metal catalysts, 2015, *J. Phys. Chem. C*, 119 (2015) 959–4966

P26) F. Karst, **M. Maestri**, H. Freund, K. Sundmacher, Reduction of Microkinetic Reaction Models for Reactor Optimization exemplified for Hydrogen Production from Methane, *Chemical Engineering Journal*, 281 (2015) 981-994

P27) T. Maffei, G. Gentile, S. Rebughini, F. Manelli, S. Lipp, A. Cuoci, **M. Maestri***, A multiregion operator-splitting CFD approach for coupling microkinetic modeling with internal porous transport in heterogeneous catalytic reactors, *Chemical Engineering Journal*, 283 (2016) 1392-1404

P28) S. Rebughini, A. Cuoci, **M. Maestri***, Handling Contact Points in Reactive CFD Simulations of Heterogeneous Catalytic Fixed Bed Reactors, *Chemical Engineering Science*, 141 (2016) 240-249

P29) A. Donazzi, M. Rahmanipour, **M. Maestri**, G. Groppi, L. Bardini, A. Pappacena, M. Boaro, Experimental and model analysis of the co-oxidative behavior of syngas feed in an Intermediate Temperature Solid Oxide Fuel Cell, *Journal of Power Sources*, 306 (2016) 467-480

P30) S. Rebughini, A. Cuoci, **M. Maestri***, Hierarchical analysis of the gas-to-particle heat and mass transfer in micro packed bed reactors, *Chemical Engineering Journal*, 289 (2016) 471–478

P31) A. Donazzi, **M. Maestri**, G. Groppi, A multistep model for the kinetic analysis of the impedance spectra of a novel mixed ionic and electronic conducting cathode, *Electrochimica Acta*, 222 (2016) 1029-1044

P32) S. Rebughini, A. Cuoci, A. G. Dixon, **M. Maestri***, Cell agglomeration algorithm for coupling microkinetic modeling and steady-state CFD simulations of catalytic reactors, *Computers and Chemical Engineering*, 97 (2017) 175-182

P33) M. Bracconi, A. Cuoci, **M. Maestri***, In-situ adaptive tabulation for the CFD simulation of heterogeneous reactors based on operator-splitting algorithm, *AIChE Journal*, 63 (2017) 95-104

P34) **M. Maestri***, Structure-dependent microkinetic modeling: Towards the nano-engineering of heterogeneous catalytic processes, *Chemistry Today*, 35 (2017) 52-53

P35) M. Bracconi, M. Ambrosetti, **M. Maestri**, G. Groppi, E. Tronconi, A systematic procedure for the virtual reconstruction of open-cell foams, *Chemical Engineering Journal*, 315 (2017) 608-620

P36) **M. Maestri***, Escaping the trap of complication and complexity in multiscale microkinetic modelling of heterogeneous catalytic processes, *ChemComm*, 53 (2017) 10244-10254 (**feature article**)

P37) Z.B. Ding, M. Tommasini, **M. Maestri***, First-principles simulation of Raman spectra of adsorbates on metal surfaces, ChemPlusChem, 82 (2017) 924-932

P38) A. Maghsoumi, A. Ravanelli, F. Consonni, F. Nanni, A. Lucotti, M. Tommasini, A. Donazzi, **M. Maestri***, Design and testing of an operando-Raman annular reactor for kinetic studies in heterogeneous catalysis, *Reaction Chemistry and Engineering*, 2 (2017) 908 - 918

P39) S. Rebughini, M. Bracconi, A.G. Dixon, **M. Maestri***, A hierarchical approach to chemical reactor engineering: an application to micro packed-bed reactors, *Reaction Chemistry and Engineering*, 2 (2018) 25-33 (**back cover**)

P40) Z. B. Ding, E. Di Marco, M. Pelucchi, T. Faravelli, **M. Maestri***, A Systematic Investigation of Hydrogen Abstraction Reactions on Graphene Edges, 2018, under review

P41) M. Bracconi, M. Ambrosetti, **M. Maestri**, G. Groppi, E. Tronconi, A fundamental analysis of the influence of the geometrical properties on the effective thermal conductivity of open-cell foams, *Chemical Engineering & Processing: Process Intensification*, 2018, accepted

P42) M. Bracconi, M. Ambrosetti, **M. Maestri**, G. Groppi, E. Tronconi, A fundamental investigation of gas/solid mass transfer in open-cell foams using a combined experimental and CFD approach, *Chemical Engineering Journal*, 2018, under review

P43) **M. Maestri*** and E. Iglesia, First-principles assessment of catalysis by confinement: NO oxidation on silicalite frameworks containing voids of molecular dimension, *Physical Chemistry Chemical Physics*, 2018, under review

P44) R. Cheula, A. Soon, **M. Maestri***, Morphological changes of catalyst materials in reacting conditions by combined ab initio thermodynamics and microkinetic modelling, *Catalysis Science and Technology*, 2018, accepted

P45) R. Uglietti, M. Bracconi, **M. Maestri***, Coupling CFD-DEM and microkinetic modelling of surface chemistry for the simulation of catalytic fluidized systems, *Reaction Chemistry and Engineering*, 2018, accepted

**INVITED TALKS**

He has delivered **44 invited talks** (24 at international conferences and workshops, 16 at international universities and research centers, 4 at international industries).

A) *International conferences, workshop and advanced schools (24)*:

1) "*Chemical reactor design and kinetic modeling for process intensification*", *Gr.I.C.U. National School of Doctorate* on "Transport Phenomena and Process Intensification", Le Castella (KR) – Italy, September 18-21, 2008.

2) *"Atomic-scale understanding of complex chemical kinetics",* Seminari del Dottorato in Ingegneria Energetica, Politecnico di Milano, May 7, 2010

3) *"Atomic-scale understanding of complex chemical kinetics",* EU-COST meeting (European Cooperation in Science and Technology) Action P-19 "*Multi-Scale Modeling of Materials*" final meeting, Imperial College, London, UK, January, 27-28, 2011

4) ***"****Atomic scale understanding of complex chemical processes through hierarchical multiscale approach",* Psi-k/CECAM Cat1P Conference (Catalysis from first-principles) 2011, Magleås, Denmark, May 22 – 26, 2011

5) "*Atomic scale understanding of complex chemical processes through hierarchical multiscale approach",* DeMiR 2011, European Workshop on Multiscale Catalytic Reactor Engineering, Technische Universität München, TUM, Garching, Germany, September 6, 2011

6) *"First-principles insights into the WGS mechanism on Rh"*, special symposium on "Steam reforming of alcohols" organized by C. Chin (U. Toronto, Canada) and K. Seshan (University Twente, The Netherlands) *15th International Congress on Catalysis* – Munich, Germany – July 1-6, 2012

7) *"Efficient Coupling Between Microkinetic Modeling and CFD: Towards a Fully First-Principles Catalytic Chemical Reaction Engineering"*, Special Session in Honor of the 2011 Wilhelm Award Winner Dionisios Vlachos, 2012 AIChE Annual Meeting, Pittsburgh, PA, USA October 28 - November 2, 2012

8) *"CatalyticFOAM, Heterogeneus catalysis within OpenFOAM",* Workshop on "HPC enabling of OpenFOAM for CFD applications, Cineca, Bologna, Italy, November 26-28, 2012

9) "*First-principles based catalytic reaction engineering*", DECHEMA-Workshop "Complex Reaction Networks: From Topological-kinetic Analysis to the Design of Industrial Reactors", Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany, January 24, 2013

10) *"Catalysts at work – from the intrinsic to the observed functionality"* Workshop on "Operando Research in Catalysis (ORCA)", organized by J. Frenken (Leiden University), S. Helveg (Haldor Topsoe), K. Reuter (TUM), Lorentz Center, Leiden University, Leiden, The Netherlands, June 24-28, 2013

11) "*Heat and mass transport in gas-solid catalytic reactors*", CECAM-Psi-kSummer School on "Basic Concepts and First-Principles Computations for Surface Science: Applications in Chemical Energy

Conversion and Storage" organized by K. Reuter (TUM, Munich) and M. Scheffler (FHI, Berlin), Waddensee, Germany, July 21-26, 2013

12) "*A first-principles approach to system complexity in heterogeneous catalysis*", Colloquium on Chemical Reaction Engineering of the European Federation of Chemical Engineering (EFCE), organized by G. Groppi, M. Maestri, E. Tronconi, Politecnico di Milano, Italy, October 17-18, 2013

13) "*Unraveling reaction mechanisms through hierarchical multiscale approaches*", CECAM Workshop on "From the chemical bond to the chemical reactor: Computational and Materials challenges in gas conversion technologies", organized by S. Piccinin (SISSA, Trieste, Italy), S. Fabris (SISSA, Trieste, Italy), L. Spanu (Shell Technology Center, Bangalore, India), S. Narasimhan (JNCASR, Bangalore, India), Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India, August 25-29, 2014

14) *"CatalyticFOAM: first principles multiscale modeling of heterogeneous catalytic reactors in openFOAM*", Workshop on "HPC enabling of OpenFOAM for CFD applications, Cineca, Bologna, Italy, March 25-28, 2015

15) *"A first principles approach two system complexity in heterogeneous catalysis*", Summer School 2015 - Helmholtz Research School for Energy-Related Catalysis, Stuttgart, Germany, July 20-24, 2015

16) *"Assessment of semi-empirical methods for hierarchical multiscale modeling of catalytic processes"*, Workshop on "Frontiers of Multi-scale Modeling in Materials, Energy & Catalysis" Castello Oldofredi Residence, Monte Isola, Italy, June 5-9, 2016

17) " *A first principles approach to system complexity in heterogeneous catalysis*", Conference on Molecular Simulation and Engineering, Politecnico di Milano, Italy, September 30, 2016

18) *"A first principles approach to system complexity in heterogeneous catalysis"*, IV congresso nazionale della Divisione della Chimica Teorica e Computazionale della Società Chimica Italiana, Scuola Normale Superiore di Pisa, Italy, October 3-5, 2016

19) "*Catalysts at work: unraveling reaction mechanisms through hierarchical multiscale approaches"*, 4th International conference on electronic materials and nanotechnology for green environment (ENGE 2016), Jeju, South Korea, November 6-9, 2016

20) *"Chemical Engineering concepts for heterogeneous catalysis"*, Workshop on "Theory of hetero-interfaces and surfaces", Yonsei University, Seoul, South Korea, November 11, 2016

21) *"Coupling detailed microkinetic modeling and CFD in heterogeneous Catalysis",* European Summer School on multiscale modeling in chemical reaction engineering", Porto Carras, Greece, Septemeber 21, 2017

22) "*A first-principles approach to system complexity in heterogeneous catalysis",* Italian Summer School on Chemical Engineering, (GriCU), Palermo, September 26, 2017

23) *"Morphological changes of catalyst materials in reacting conditions by combined ab-initio thermodynamics and microkinetic modeling."*, 7th Bonn Humboldt Award Winners' Forum "Fundamental Concepts and Principles of Chemical Energy Conversion", Bonn, October 11-15, 2017

24) "*Design of rupture disks for runaway reactions: comparison between short-cut and dynamic methods"*, IoIQ Workshop on process safety, Hilton Post Oak, Houston, TX, USA January 29, 2018

B) *Invited seminars in international universities and research centers (16)*:

25) *"Atomic-scale understanding of complex chemical processes",* Guest lecture, Max Planck Institute for Dynamics of Complex Technical Systems (host: Prof. Dr. Kai Sundmacher), Magdeburg, Germany, February 3, 2011

26) **"***Atomic scale understanding of complex chemical processes at surfaces"*, Guest lecture, Karlsruhe Institute of Technology, KIT (host: Prof. Dr. Olaf Deutschmann), Karlsruhe, Germany, July 15, 2011

27) *"Efficient coupling between microkinetic modeling and CFD: towards a fully first-principles catalytic chemical reaction engineering"*, Lehrstuhl für Theoretische Chemie, Technische Universität München, TUM, Garching, Germany, October 24, 2011

28) *"First-principles-based catalytic reaction engineering",* Laboratory for Chemical Technology, Universiteit Gent (host: Prof. Dr. Guy B. Marin), Gent, Belgium, September 7, 2012

29) "*Atomic scale understanding of complex chemical processes through hierarchical multiscale approach",* University of Houston (host: Prof. Dr. Jeff Rimer), Department of Chemical and Biological Engineering, Houston, TX, USA, January 11, 2012

30) *"Bringing microkinetic modeling up to the real world: a first-principles approach to system complexity in heterogeneous catalysis"*, University of Houston (host: Prof. Dr. Lars Grabow), Department of Chemical and Biological Engineering, Houston, TX, USA, January 29, 2013

31) "*A first-principles approach to system complexity in heterogeneous catalysis*", UniCat – Unifying concepts in catalysis, TU Berlin – Gerhard Ertl Center (host: Prof. Dr. M. Driess), Berlin, Germany, September 16, 2013

32) "*A first-principles approach to system complexity in heterogeneous catalysis*", University of Pittsburgh (host: Prof. Dr. Giannis Mpourmpakis), Department of Chemical Engineering, Pittsburgh, PA, USA, February 1, 2014

33) "*A first-principles approach to system complexity in heterogeneous catalysis*", University of Delaware (host: Prof. Dr. D.G. Vlachos), Department of Chemical Engineering and Center for Catalytic Science and Technology, Newark, DE, USA, February 3, 2014

34) "*Unraveling reaction mechanisms through hierarchical multiscale approaches*", UniCat – Unifying concepts in catalysis, TU Berlin – Gerhard Ertl Center (host: Prof. Dr. P. Hildebrandt), Berlin, Germany, March 26, 2014

35) "*First-Principles Chemical Engineering: towards Functional-based Process Intensification",* TU Berlin. Process Engineering Department (Host: Prof. Dr. R. King), Berlin, Germany, November 24, 2014

36) "Mechanistic insights into the $CO_2$ activation on metal surfaces", University of Houston (host: Prof. Dr. Bill Epling), Department of Chemical and Biological Engineering, Houston, TX, USA, January 28, 2015

37) "*A first-principles approach to system complexity in heterogeneous catalysis*", Worcester Polytechnic Institute (host: Prof. Dr. A.G. Dixon), Department of Chemical Engineering, Worcester, MA, USA, January 22, 2016

38) "*A first-principles approach to system complexity in heterogeneous catalysis*", Politecnico di Torino (host: Prof. Dr. D. Marchisio), Torino, Italy, May 18, 2017

39) "*Escaping the trap of complication and complexity in multiscale microkinetic modelling of heterogeneous catalytic processes"* (host: Dr. Gonzalo Prieto), Max-Planck-Institut für Kohlenforschung - Mülheim, Germany, February 12, 2018

40) *"Structure-dependent microkinetic modeling: methodology and applications"*, Pregl Colloquium, National Institute of Chemistry, Lubiana, Slovenia, March 22, 2018

C) <u>*Invited seminars in industrial research centers (4)*</u>:

41) *"Microkinetic models: reaction/reactor engineering"*, ENI s.p.a., workshop on *"Experiences in short contact time catalytic phenomena for producing synthesis gas and $H_2$ from hydrocarbons and other compounds from biomass"*, San Donato Milanese (MI), Italy, March 20, 2009

42) "*Atomic scale understanding of complex chemical processes through hierarchical multiscale approach",* TOTAL S.A. (host: Dr. Daniel Curulla-Ferre), Paris, France, December 12, 2011

43) *"Emergency Relief Systems for Runaway Reactions: Concepts and Design"*, JACOBS Engineering (host: Dr. Ing. Lorenzo Pirovano), Milan, Italy, April 19, 2012

44) *"Handling complex homogeneous and heterogeneous kinetic schemes in the detailed simulation of gas-solid catalytic reactor"*, Shell Technology Center – Webinar: Houston, USA; Bangalore, India; Amsterdam, ND (host: Dr. Leonardo Spanu, Shell Technology Center, Bangalore), October 27, 2014

He has also delivered > **60 oral contributed presentations at international conferences** and **20 poster presentations**.