# MATTEO MAESTRI

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## 1. EDUCATION

Politecnico di Milano, Italy, 2008
Ph. D. *cum laude* (highest grade) in Chemical Engineering and Industrial Chemistry

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

## 2. RESEARCH EXPERIENCE

Full Professor
Politecnico di Milano, Italy, 2019 – present

Group leader of the ERC Research Group SHAPE (http://www.shape.polimi.it),
Politecnico di Milano, Italy, 2016 – present

Associate Professor
Politecnico di Milano, Italy, 2015 – 2019

Assistant Professor
Politecnico di Milano, Italy, 2008 – 2015

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

## 3. 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

## 4. TEACHING ACTIVITY

Professor of *Advanced Catalytic Reactor Design* – 5 CFU, 2011 – present
Graduate, Chemical Engineering, Politecnico di Milano
(subject: transport phenomena in reacting systems, catalysis and catalytic reactor design)
Evaluation from students: high (maximum grade)

Professor of *Fundamentals of Chemical Processes*– 8 CFU, 2018 – present
Graduate, Energy Engineering, Politecnico di Milano
(subject: chemical kinetics, thermodynamics, mass and energy balances, process analysis and design)
Evaluation from students: n/a (course will start in Sept 2018)

Professor of *Petroleoum Technology and Biofuels* – 8 CFU, 2016 – 2018
Graduate, Energy Engineering, Politecnico di Milano
(subject: oil refinery, biorefinery)
Evaluation from students: high (maximum grade)

Professor of *Fundamentals of Chemical Processes for Energy and Environment* – 5 CFU, 2015 – 2016
Graduate, Energy Engineering, Politecnico di Milano
(subject: chemical kinetics, thermodynamics, mass and energy balances, process analysis and design)
Evaluation from students: high (maximum grade)

Professor of *Fondamenti dell'industria di processo* – 5 CFU, 2010 – 2011
Graduate, Ingegneria della prevenzione e della sicurezza, Politecnico di Milano
(subject: mass and energy balances, process analysis and design)
Evaluation from students: high (maximum grade)

I have also given several short-courses in industries and Ph.D. Schools as specified in *Section 13 "Invited Talks"* of this CV.

I am also co-authoring (together with Dion Vlachos, Preeti Aghalayam, Niket Kaisare, Alberto Cuoci) a book on multiscale modelling of heterogeneous catalytic systems (*Reaction Engineering of Heterogeneous Catalytic Systems*) for Elsevier.

## 5. SUPERVISION OF STUDENTS AND RESEARCH FELLOWS

Since 2011, I have supervised:

a) 3 Post-doctoral researchers (2 completed, 1 in progress)
b) 5 PhD Students (2 completed, 3 in progress) in Chemical Engineering at Politecnico di Milano, Italy;
c) 44 (31 completed, 13 in progress) Master students in Chemical Engineering/Energy Engineering at Politecnico di Milano, Italy.

PhD students and Post-doctoral fellows are now employed in Casale (Lugano, Switzerland), BASF (Bologna), Saes Getters (Milano) and Sharif University of Technology (Iran).

Currently, my ERC group consists of 1 senior researcher (selection in progress), 1 Senior Researcher, 2 Post-doctoral fellows, 3 Ph.D. Students, 13 Master students.

## 6. RESEARCH INTERESTS

During my research activity, I have 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. Recently, **I have also developed experimental expertise in the development and analysis of operando experiments for kinetic studies in heterogeneous catalysis**.

My main research interests are:

i. Chemical and catalytic reactor engineering.
ii. First principles multiscale modeling of catalytic chemical processes.
iii. Microkinetic modeling and analysis.
iv. Computational fluid dynamics of reacting flows.
v. Electronic structure calculations (DFT) of materials and reaction pathways.
vi. Kinetic-Monte-Carlo simulations.
vii. Operando-Raman kinetic experiments.

## 7. HONORS/AWARDS

- 2018: selected for the *Reaction Chemistry and Engineering* "2019 Emerging Investigators special issue", Royal Society of Chemistry
- 2018: Pregl Lecture, Kemijski inštitut, National Institute of Chemistry – Ljubljana, Slovenia
- 2017: Listed in the selection of Italy's best under-40 researchers currently active both in Italy and abroad, *CARTADITALIA - Istituto Italiano di Cultura*, Brussels
- 2016: selected for a Feature Article in *Chemical Communications*, Royal Society of Chemistry
- - ERC, European Research Council
- 2016. selected for the Early Career Series of *ChemPlusChem*, Wiley
- 2015: SIR (Scientific Independence of Young Researchers) - MIUR, Rome
- 2012: *Young Scientist Award* at the 15$^{th}$ International Congress on Catalysis (Munich, Germany, July 1-6, 2012), presented by the International Association of Catalysis Societies (IACS).
- 2010: *Young Researcher Award* at the 21$^{st}$ International Symposium on Chemical Reaction Engineer (ISCRE), June 13-16, 2010, Philadelphia, USA
- 2009: *Alexander von Humboldt Research Fellowship*
- 2008: *Young Scientist Award* at the 14$^{th}$ International Congress on Catalysis (Seoul, Korea, July 13-18, 2008), presented by the International Association of Catalysis Societies (IACS).

Moreover, I have given 52 invited talks at international conferences, workshops and industrial meeting as detailed in the *Section 13 "Invited Talks"* of this CV.

## 8. SCIENTIFIC SERVICES AND COMMISSIONS OF TRUST

*a) Co-organized workshops and conferences*:

1. organizer (together with R. Horn and K. Reuter) of *DeMiR 2011: From Detailed Microkinetics to the Reactor*, European Workshop on Multiscale Catalytic Reactor Engineering, TUM, Munich, Sept. 6, 2011
2. organizer (together with G. Groppi and E. Tronconi) of *Colloquium on Chemical Reaction Engineering 2013* – sponsored by the European Federation of Chemical Engineering (EFCE): "First-principles methods in Chemical Reaction Engineering", 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), 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
7. organizer (together with R. Cheula and G. Moroni, Politecnico di Milano) of the workshop on "Structure dependent microkinetic modeling: theory and experiments", Castello Oldofredi, Monte Isola, Brescia, June 13-15, 2018

*b) Reviewer for the following scientific journals (*Publons profile: https://publons.com/a/1301801*)*:

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

*c) Reviewer for the following research foundations and agencies*:

- 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)

## 9. MAJOR SCIENTIFIC COLLABORATIONS

- *Prof. Alberto Cuoci* – Politecnico di Milano, Italy – Topic: "CFD simulations of chemically reacting flows at surfaces" (9 joint papers published).
- *Prof. Anthony G. Dixon* – Worcester Polytechnic Institute, Worcester, MA, USA – Topic: "Numerical methods for the computational fluid dynamics of catalytic reactors" (2 joint papers published).
- *Prof. Enrique Iglesia* – University of California, Berkeley, USA – Topic: "First-principles assessment of catalysis by confinement in microporous siliceous zeolites" (1 joint paper published).
- *Dr. Simone Piccinin* – CNR-SISSA, Trieste, Italy – Topic: "First principles assessment of $CO_2$ activation pathways on metal supported catalysts" (1 joint paper published).

- *Prof. Matteo Pasquali* – Rice University, Houston, USA – Topic: "Numerical modelling of particle growth in fluidized bed reactors for production of carbon-nanotubes" (1 research project under evaluation).
- *Prof. Karsten Reuter* – Technische Universität München, Germany – Topic: "Coupling kinetic Monte Carlo simulations with CFD in catalysis" (3 joint papers published).
- *Prof. Kai Sundmacher* – Max-Planck-Institut, Magdeburg, Germany – Topic: "Advanced optimization of catalytic reactors using microkinetic modeling" (2 joint papers published).
- *Prof. Matteo Tommasini* – Politecnico di Milano, Italy – Topic: "Raman spectroscopy of catalyst materials" – (2 joint papers published).
- *Prof. Dion Vlachos* – University of Delaware, Newark, USA – Topic: "Microkinetic modelling of complex systems" (7 joint papers published).

## 10. RESEARCH GRANTS

I am the **principal investigator** of research projects for a total budget **in excess of 2,000,000 Euro** and **in excess of 30 Million cpu-hours** at national and international supercomputing centres.

*Peer-reviewed research projects as Principal Investigator*:

- ***H2020-MSCA-IF-EF-ST-2018*** (Marie-Sklodowska-Curie Actions Individual Fellowship) – Progetto: Biogas2Syngas – November 2019 – November 2021
- ***H2020-MSCA-IF-EF-ST-2018*** (Marie-Sklodowska-Curie Actions Individual Fellowship) – Progetto EmPHaTHY - November 2019 – November 2021
- ***H2020 – Call: H2020-NMBP-TO-IND-2018-2020*** - Software Platform for Multiscale Modelling of Reactive Materials and Processes (ReaxPro) – Evaluation at the second stage (first stage successfully passed) – Duration: 48 months – Total Grant: 4,114,410 Euro (Grant for PoliMI: 329,625 Euro) – Role: Coordinator of the PoliMI unit
- ***Department of Energy, USA – Call: ARPA-E*** – "Converting hydrocarbons to recyclable lightweight automotive structures with positive hydrogen power output" (Coordinator: Prof. Matteo Pasquali – Rice University, Houston, TX, US) – Evaluation at the second stage (first stage successfully passed) – Duration: 36 months –Subgrant for PoliMI: 90,000 US Dollars – Role: Coordinator of the PoliMI subunit
- ***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**
- ***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**

*Peer-reviewed research projects for computational time as Principal Investigator:*

- ***CINECA Supercomputing Centre (Bologna, Italy)*** – project: SPIRE – THEORETICAL STUDY OF C AND S POISONING DURING THE DRY REFORMING OF METHANE – from February 2018 to February 2019 (ISCRA B CALL 2017) – Grant: **4 Million CPU hours**
- ***CINECA Supercomputing Centre (Bologna, Italy)*** – project: AURORA – THEORETICAL EVALUATION OF REACTION PATHWAYS RELEVANT TO CVD– from August 2017 to August 2018 (ISCRA B CALL 2017) – Grant: **600,000 CPU hours**
- ***CINECA Supercomputing Centre (Bologna, Italy)*** – project: CO2Act – ASSESSMENT OF CATALYST DESCRIPTORS FOR THE $CO_2$ ACTIVATION ON LOW INDEX METALLIC SURFACES– from July 2016 to July 2017 (ISCRA B CALL 2016) – Grant: **600,000 CPU hours**
- ***CINECA Supercomputing Centre (Bologna, Italy)*** – project: MASSFOAM - CFD MODELING OF EXTERNAL MASS TRANSFER IN OPEN-CELL FOAMS FOR ADVANCED REACTOR DESIGN (LISA CALL 2016) – from December 2016 to November 2017 – Grant: **600,000 CPU hours**
- ***CINECA Supercomputing Centre (Bologna, Italy)*** – project: PROSPECT - ASSESSMENT OF CATALYST DESCRIPTORS FOR THE $CO_2$ ACTIVATION ON LOW INDEX METALLIC SURFACES – from May 2016 to February 2017 (ISCRA C CALL 2016) – Grant: **80,000 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 B 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 December 2013 (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 as Principal Investigator*:

I have been/am the **Principal Investigator** for several research project for industry in the last 6 years:

- 2012: BASF (Ludwigshafen, Germany) – Topic: *Computational fluid dynamics of heterogeneous catalytic reactors*
- 2012: BASF (Ludwigshafen, Germany) - Topic: *Advanced modeling of heterogeneous catalytic reactors*
- 2013: BASF (Ludwigshafen, Germany) - Topic: *Advanced modeling of heterogeneous catalytic reactors*
- 2014: VDI TECHNOLOGIEZENTRUM GmbH (EUROKIN) - Topic: *Simulation of spatially-resolved diffusion and reaction data*

- 2016: SHELL (Amsterdam, The Netherlands) - Topic: *Multiscale modeling of heterogeneous catalytic reactors*
- 2016: VDI TECHNOLOGIEZENTRUM GmbH (EUROKIN) - Topic: *Simulation of spatially-resolved diffusion and reaction data: Case studies regarding diffusion and reaction -*
- 2017: SHELL (Bangalore, India) – Topic: *Multiscale simulations of gas-solid catalytic reactors: extension to fluidization and intraphase transport phenomena*

## 12. RESEARCH PUBLICATION TRACK-RECORD

I am author/co-author of 54 international scientific papers in peer-reviewed journals or book-chapters (16 as first author; 24 as corresponding author; 3 as single author; Orcid ID: http://orcid.org/0000-0002-8925-3869).

I am also co-authoring (together with Dion Vlachos, Preeti Aghalayam, Niket Kaisare, Alberto Cuoci) a book on multiscale modelling of heterogeneous catalytic systems (*Reaction Engineering of Heterogeneous Catalytic Systems*) for Elsevier.

*Publication highlights (numbers refer to the list of scientific publications given in Section 15 of this CV)*:

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 featured in the **VIP (Very Important Publication) collection**

vi. P15 in *Angewandte Chemie Int. Ed.* was featured in the **cover picture**

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* was featured in ***ACS Editors' Choice***

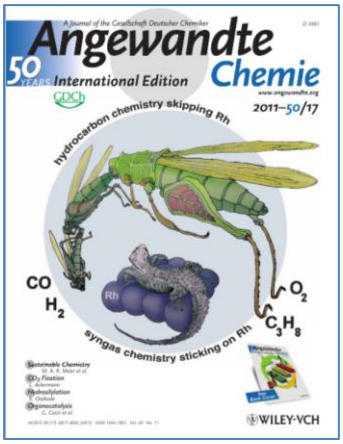
x. P38 in *A.I.Ch.E. Journal* was featured in ***Editor's Choice: Reaction Engineering, Kinetics and Catalysis***

xi. P45 in *Reaction Chemistry and Engineering* was selected for the **inside front cover**

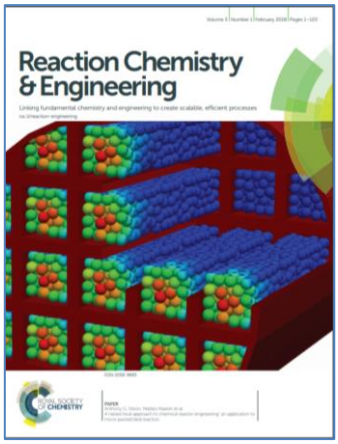
xii. P46 in *Chemical Engineering & Processing: Process Intensification* was included in the Top25 hottest articles list (most downloaded) of Chemical Engineering & Processing: Process Intensification for the period July - September 2018

xiii. P48 in *Catalysis Science and Technology* was featured in the **inside front cover**

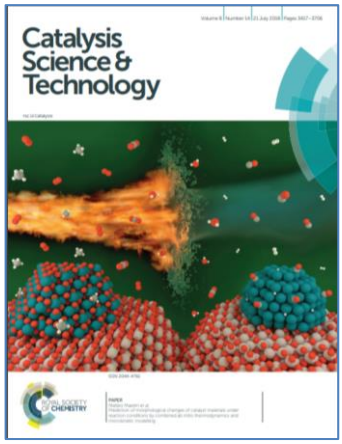
xiv. P48 in *Catalysis Science and Technology* was featured in the Themed collection of Catalysis Science and Technology "***2018 Catalysis Science & Technology HOT Articles***"




*Front Cover – Angwandte Chemie International Edition (P15)*




*Inside Front Cover – Reaction Chemistry and Engineering (P45)*




*Inside Front Cover – Catalysis Science and Technology (P48)*

**Patent application**

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

## 13. INVITED TALKS

A) *International conferences, workshop and advanced schools (26)*:

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

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

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

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

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

23) **M. Maestri**, *"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) **M. Maestri**, "*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

25) **M. Maestri**, "*Kinetic analysis of methane dry reforming on Rh in operando-Raman annular reactor*" ACS National meeting, Special Symposium on Operando Analysis in Catalysis, Boston, MA, US, August 19-23, 2018

26) **M. Maestri**, "*Prediction of morphological changes of catalyst materials for structure-dependent-microkinetic analysis*", Workshop on "Kinetic, Transport Modelling and Experiments in Catalytic Systems", IchemE, University College London, September 19, 2018

27) **M. Maestri**, *"Structure-dependent microkinetic analysis of heterogeneous catalytic processes: methodology and applications"*, Workshop on "Multiscale aspects of heterogeneous catalytic processes", University of Stuttgart, Germany, November 21, 2018

B) *Invited seminars in international universities and research centers (19)*:

28) **M. Maestri**, *"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

29) **M. Maestri**, *"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

30) **M. Maestri**, *"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

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

32) **M. Maestri**, "*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

33) **M. Maestri**, *"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

34) **M. Maestri**, "*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

35) **M. Maestri**, "*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

36) **M. Maestri**, "*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

37) **M. Maestri**, "*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

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

39) **M. Maestri**, "*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

40) **M. Maestri**, "*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

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

42) **M. Maestri**, "*A first-principles approach to system complexity in heterogeneous catalysis*", Rice University (host: Prof. Dr. Matteo Pasquali), Department of Chemical Engineering, Houston, TX, US, June 2, 2017

43) **M. Maestri**, "*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

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

45) **M. Maestri**, *"Structure-dependent microkinetic analysis of heterogeneous catalytic processes: methodology and applications"*, University of Pittsburgh (host: Prof. Dr. Giannis Mpourmpakis), Department of Chemical Engineering, Pittsburgh, PA, USA, August 27, 2018

46) **M. Maestri**, *"Structure-dependent microkinetic analysis of heterogeneous catalytic processes: methodology and applications"*, University of Delaware (host: Prof. Dr. D.G. Vlachos), Delaware Energy Institute, Newark, DE, USA, August 28, 2018

47) **M. Maestri**, *"Structure-dependent microkinetic analysis of heterogeneous catalytic processes: methodology and applications"*, University of Houston (host: Prof. Dr. J. Rimer), Houston, TX, USA, January 30, 2019

48) **M. Maestri**, *"Structure-dependent microkinetic analysis of heterogeneous catalytic processes: methodology and applications"*, Norwegian University of Technology (host: Prof. Dr. De Chen), Trondheim, Norway, March 5, 2019

C) *Invited seminars in industrial research centers (7)*:

49) **M. Maestri**, *"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

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

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

52) **M. Maestri**, *"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

53) **M. Maestri**, *"An integrated theoretical-experimental multiscale methodology for the application of "theory" in applied catalysis",* Shell Technology Center (host: Dr. Leonardo Spanu), Houston, TX, US, January 25, 2017

54) **M. Maestri**, *"Structure-dependent microkinetic modeling: methodology and applications"*, Johnson Matthey (host: Dr. Andrew York), Sonning, Common, UK, June 20, 2018

55) **M. Maestri,** *"Fundamental concepts of biofuel technologies"*, Scientific course for SAIPEM employees, 10 hours, September – October 2018, SAIPEM, San Donato Milanese, Italy

I am also the author/co-author of several communications presented at national and international conferences, where I have given **more than 70 oral contributed presentations at international conferences** and **20 poster presentations**. The international conferences in the field of catalysis and chemical reaction engineering in which I regularly participate are: Europacat, ICC (International Congress on Catalysis), NGCS (Natural Gas Symposium Series), NAM meetings (North American Catalysis Society meetings), ISCRE meetings (International Symposium of Chemical Reaction Engineering) and ACS meetings.

## 14. LIST OF SCIENTIFIC PEER-REVIEWED PUBLICATIONS

"*" indicates when I am the 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) 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

P3) **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.

P4) 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.

P5) 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.

P6) 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.

P7) **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.

P8) **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

P9) **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.

P10) **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

P11) 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

P12) **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.

P13) **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

P14) 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

P15) 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

P16) **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

P17) 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 + selected for cover picture**)

P18) 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

P19) 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

P20) **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

P21) 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

P22) **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 (**invited book chapter**)

P23) **M. Maestri*** and A. Cuoci, Coupling CFD with detailed microkinetic modeling in heterogeneous catalysis, *Chemical Engineering Science*, 96 (2013) 106-117

P24) 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

P25) 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

P26) **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

P27) 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 - special issue edited by M. Nilles, BASF and G. Wozny, TU- Berlin**)

P28) S. Matera, **M. Maestri***, A. Cuoci, K. Reuter, Predictive-quality surface reaction chemistry in real reactor models: integrating first-principles kinetic Monte Carlo simulations into computational fluid dynamics, *ACS Catalysis*, 4 (2014) 4081–4092 (**featured in *ACS Editor's Choice***)

P29) 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

P30) L. Dietz, S. Piccinin, **M. Maestri***, Mechanistic insights into CO2 activation via reverse water-gas shift on metal surfaces, 2015, *J. Phys. Chem. C*, 119 (2015) 4959–4966

P31) 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

P32) T. Maffei, G. Gentile, S. Rebughini, M. Bracconi, 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

P33) 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

P34) 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

P35) 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

P36) 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

P37) 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

P38) 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 (**featured in *Editor's Choice: Reaction Engineering, Kinetics and Catalysis***)

P39) **M. Maestri***, Structure-dependent microkinetic modeling: Towards the nano-engineering of heterogeneous catalytic processes, *Chemistry Today*, 35 (2017) 52-53

P40) 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

P41) **M. Maestri***, Escaping the trap of complication and complexity in multiscale microkinetic modelling of heterogeneous catalytic processes, *Chemical Communications* 53 (2017) 10244-10254 (**invited feature article**)

P42) Z.B. Ding, M. Tommasini, **M. Maestri***, First-principles simulation of Raman spectra of adsorbates on metal surfaces, ChemPlusChem, 82 (2017) 924-932 (**invited – Early Carrier Series**)

P43) 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

P44) 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 (**invited book chapter**)

P45) 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*, 3 (2018) 25-33 (**selected for inside front cover**)

P46) 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*, 129 (2018) 181-189

P47) 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*, 352 (2018) 558-571

P48) R. Cheula, A. Soon, **M. Maestri***, Prediction of morphological changes of catalyst materials in reacting conditions by combined ab initio thermodynamics and microkinetic modelling, *Catalysis Science and Technology*, 8 (2018) 3493-3503 (**selected for inside front cover + selected for the special themed collection "2018 Catalysis Science & Technology HOT Articles"**)

P49) 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*, 3 (2018) 527-539

P50) **M. Maestri*** and E. Iglesia, First-principles theoretical assessment of catalysis by confinement: NO-$O_2$ reactions within voids of molecular dimensions in siliceous crystalline frameworks, *Physical Chemistry Chemical Physics*, 20 (2018) 15725-15735

P51) Z. B. Ding, E. Di Marco, M. Pelucchi, T. Faravelli, **M. Maestri***, First-principles assessment of the analogy between gas phase and gas-solid H-abstraction reactions at graphene edges, 2019, *Chemical Engineering Journal*, in press, doi.org/10.1016/j.cej.2018.08.077

P52) M. Bracconi, M. Ambrosetti, O. Okafor, V. Sans, X. Ou, C. Pereira Da Fonte, X. Fan, **M. Maestri**, G. Groppi, E. Tronconi, Investigation of pressure drop in 3D replicated open-cell foams: coupling CFD with experimental data on additively manufactured foams, 2019, *Chemical Engineering Journal*, in press, 10.1016/j.cej.2018.10.060

P53) Z.B. Ding, M. Tommasini, and **M. Maestri***, "A topological model for predicting adsorption energies of polycyclic aromatic hydrocarbons on late-transition metal surfaces", *Reaction Chemistry and Engineering*, 4 (2019) 410-417

P54) Z.B. Ding and **M. Maestri***, "First-principles assessment of BEP relations for structure-dependent microkinetic modeling in heterogeneous catalysis", 2019, Industrial & Engineering Chemistry Research, accepted