# Carla Maria Coppola: *curriculum vitae*

**March 7, 2018**

**Personal**

Born in Bari, Italy, 3 April 1982. Citizenship: Italian

Dept. of Chemistry
University of Bari
Via Orabona, 4
70124 Bari, Italy
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**Academic Positions**

Researcher, $4^{th}$ January 2016 – present

Research Assistant, $1^{st}$ June 2011 – $31^{st}$ May 2015
University of Bari, Chemistry Department
"Elementary processes and kinetics of hydrogen-helium plasma in hypersonic re-entry in Jupiter atmosphere"

Hononary Research Associate, August 2010 – July 2011
University College London - Physics & Astronomy Department
"Electron-molecule scattering in Early Universe"

PhD student, 2007 – 2010
University of Bari, Department of Chemistry

**Education**

Ph.D. in Chemical Sciences
University of Bari - Chemistry Department & Osservatorio Astrofisico di Arcetri
$30^{th}$ March 2010
Dissertation: *Vibrational distribution function of $H_2$ and $H_2^+$ in the Primordial Universe chemistry*, supervised by Proff. Savino Longo, Daniele Galli & Francesco Palla

M.A. in Theoretical Physics
University of Bari, $26^{th}$ October 2006
Dissertation: *Molecular hydrogen kinetics in the primordial Universe*
110/110 cum laude
supervised by Prof. Savino Longo

A.B. in Physics
University of Bari, $23^{rd}$ July 2004 Dissertation: *Classical motion of a relativistic string and introduction to its quantum aspects*
110/110 cum laude
supervised by Prof. Maurizio Gasperini

**Refereed Publications**

1. C. M. Coppola, M. V. Kazandjian, D. Galli, A. N. Heays, E. F. van Dishoeck, "Non-thermal photons and direct photodissociation of H2, HD and HeH+ in the

chemistry of the primordial Universe", 2017, MNRAS, 470, 4, 41634167

2. Sidaty Cheikh Sid Ely, C. M. Coppola, F. Lique, "State-to-state study of the D+H2(v = 0, j) collisions and its astrophysical application", 2017, MNRAS, 466, 2, 2175-2180

3. M. V. Kazandjian, I. Pelupessy, R. Meijerink, F. P. Israel , C. M. Coppola, M. J. F. Rosenberg, M. Spaans, "Constraining Cloud Parameters Using High Density Gas Tracers in Galaxies", 2016, A&A, 595, A124-A137

4. C. M. Coppola, G. Mizzi, D. Bruno, D. Galli, S. Longo, F. Palla, "State-to-state chemistry of $H_2$ and $H_2^+$ and post-shock conditions in primordial composition gas", 2016, *MNRAS*, 457, 4, 3732-3742

5. K. Sugimura, C. M. Coppola, D. Galli, F. Palla, K. Omukai, "Role of the $H_2^+$ channel in the primordial star formation under strong radiation field and the critical intensity for the supermassive star formation", 2016, *MNRAS*, 456, 1, 270-277

6. F. Esposito, C. M. Coppola, D. De Fazio, "Complementarity between Quantum and Classical Mechanics in Chemical Modeling. The H + $HeH^+ \rightarrow H_2^+$ + He Reaction: A Rigourous Test for Reaction Dynamics Methods", 2015, *The Journal of Physical Chemistry A*, 119, 51, 12615-12626

7. A. Damone, A. Panarese, C. M. Coppola, J. Jansky, C. Coletti, L. Chiodo, G. Serianni, V. Antoni, S. Longo, "Theoretical determination of the microstructure of Cs covering of Mo in negative ion sources for Nuclear Fusion applications", 2015, *Plasma Physics and Controlled Fusion* , 57, 035005 (article chosen to be published on the cover page for the Volume 57 Number 3)

8. S. Longo, P. Diomede, A. Damone, C. M. Coppola, J. Jansky, A. Panarese, A. Laricchiuta, F. Esposito, O. De Pascale, F. Taccogna, P. Minelli, C. Coletti, C. Gorse, M. Capitelli, G. Serianni, V. Antoni, "Cold plasmas and molecular aspects in fusion energy", 2013, Conference book "The Terawatt challenge", edited by Accademia dei Lincei

9. S. Longo, C. M. Coppola, " Stochastic models of chiral symmetry breaking in autocatalytic networks withanomalous fluctuations", 2013, *Rend. Fis. Acc. Lincei*, DOI 10.1007/s12210-013-0234-4

10. C. M. Coppola, D. Galli, F. Palla, S. Longo & Jens Chluba, 2012, "Non-thermal photons and $H_2$ formation in the early Universe", 2013, *MNRAS*, 434, 1, 114-122

11. C. M. Coppola, R. D'Introno, D. Galli, J. Tennyson, S. Longo, "Non-equilibrium $H_2$ formation in the early Universe: energy exchanges, rate coefficients and spectral distortions.", 2012, *The Astrophysical Journal Supplement*, 199, 16

12. C. M. Coppola, L. Lodi, J. Tennyson, "Radiative cooling functions for primordial molecules.", 2011, *MNRAS*, 415, 1, 487

13. S. Longo, C. M. Coppola, D. Galli, F. Palla, M. Capitelli, "The role of vibrationally excited molecules in the chemistry of the Early Universe - Molecular hydrogen and its cation.", 2011, *Rendiconti Lincei*, 22, 119
14. C. M. Coppola, S. Longo, M. Capitelli, F. Palla, D. Galli, "Vibrational level population of $H_2$ and $H_2^+$ in the early Universe.", 2011, *The Astrophysical Journal Supplement*, 193, 7
15. M. Capitelli, D. Bruno, C. Catalfamo, R. Celiberto, G. Colonna, C.M. Coppola, G. D'ammando, P. Diomede, F. Esposito, C. Gorse, A. Laricchiuta, S. Longo, F. Taccogna
"Elementary processes, thermodynamics and transport of $H_2$ plasmas", 2011, *Atomic and plasma-material interaction data for fusion*, 16, 29-47
16. C. M. Coppola, P. Diomede, S. Longo, M. Capitelli, "$H_2$ and HD direct photodissociation in the chemistry of primordial Universe.", 2011, *The Astrophysical Journal*, 727, 1, 37
17. M. Capitelli, C.M. Coppola, P. Diomede, S. Longo, "An evaluation of the effect of the dissociative attachment of vibrationally excited $H_2$ on primordial universe chemistry.", 2007, *Astronomy & Astrophysics*, 470, 811

**Presentations**

"Energy exchanges in hydrogen-rich systems: high-temperature vs. low temperature cases (and high densities vs. low densities cases)" [Invited] 2017
*Processus physico-chimiques d'interet astrophysique*
Bastia, $12^{th}$-$15^{th}$ June 2017

"State-to-state study of the D+H2(v=0,j) collisions and their astrophysical implications" 2017
*The Astrochemical week*
Faro, $17^{th}$-$19^{th}$ January 2017

"$H_2^+$ Chemistry and Direct Collapse Black Hole Formation in the Early Universe" 2016
*International Meeting on Atomic and Molecular Physics and Chemistry*
Le Havre, $27^{th}$-$30^{th}$ June, 2016

"Systems of ODEs in applied sciences: the case of chemical kinetics in the early Universe" [Invited] 2016
*Workshop on numerical methods for multi-parametric Boundary Value Problems*
Bari, $2^{nd}$-$5^{th}$ February, 2016

"Non-equilibrium $H_2$ and $H_2^+$ kinetics in the early Universe chemistry and in primordial star formation" [seminar, invited] 2015
Le Havre, $3^{rd}$ December 2015

"Non equilibrium aspects of molecular hydrogen plasmas" [Invited] 2015
*European Plasma Society*
Lisbon, $22^{nd}$-$26^{th}$ June 2015

"Photodissociation of $H_2$ and HD in a non-thermal radiation background: application to the early Universe chemistry" [Invited] 2015

*Photodissociation in Astrochemistry*
Leiden, $3^{rd}$-$5^{th}$ February 2015

"Simulazione al computer del mezzo interstellare primordiale" 2014
*Materia extraterrestre ed esplorazione dello Spazio*
Bari, $12^{th}$ November 2014

"Primordial $H_2$ formation in the early Universe" [seminar, invited] 2014
Trieste, 15 October 2014

"Chemistry in pregalactic shocks: a state-to-state approach" [Invited] 2014
*III Workshop on Active Galactic Nuclei and Gravitational Lensing*
Končarevo (Serbia), $7^{th}$-$11^{th}$ October 2014

"Chemical data for astrophysical applications: an overview" [Invited] 2014
*Quantum Days in Bilbao*
Bilbao, $15^{th}$-$16^{th}$ July

"State-to-state resolved chemistry in hydrogen plasma for astrophysical application", 2014
*European Plasma Society*
Berlin, $23^{rd}$-$28^{th}$ June

"Out of equilibrium: the interesting case of early Universe chemistry", 2012
*The low-metallicity ISM: Chemistry, turbulence and magnetic fields*
Georg-August-Universität, Göttingen, $8^{th}$-$13^{th}$ October

"Atomic and molecular processes: non-thermal photons and the chemistry of primordial Universe" [Invited] 2012
*Theoretical and computational astrochemistry*, CECAM workshop
Scuola Normale Superiore, Pisa, $30^{th}$ August-$1^{st}$ September

"Molecular kinetics and cooling in the primordial Universe" [Invited] 2012
*Data and models for the chemistry of the early Universe*
Arcetri, $6^{th}$-$7^{th}$ February 2012

"Non-equilibrium vibrational distributions and energy exchange processes in the Early Universe." [Invited] 2011
*The chemical Cosmos, Annual Conference*
Malta, $12^{th}$-$14^{th}$ October 2011

**Other Publications**

J. Zs. Mezei, F. Colboc, D. O. Kashinsky, D. A. Little, M. D. Epee Epee, S. Niyonzima, N. Pop, C. M. Coppola, K. Chakrabarti, O. Motapon, A. Bultel , K. Hassouni, D. Talbi, A. P. Hickman, A. Faure, J. Tennyson, and I. F. Schneider "Recombination, excitation and dissociation of hydride molecular cations in low energy electron collisions"
Contributed talk to the conference "Hydrides toolbox", Paris, $12^{th}$-$15^{th}$ December 2016

K. Sugimura, C. M. Coppola, K. Omukai, D. Galli, F. Palla
"Conditions for Direct Collapse Black Hole Formation with Detailed Microphysics"
Poster contribution at Stars V conference, Heidelberg, $1^{st}$-$5^{th}$ August 2016

J. Zsolt Mezei, F. Colboc, C. M. Coppola, O. Motapon, C. Jungen, I. F. Schneider
"Elementary processes involving $H_2^+$ from early Universe towards star formation"
Poster contribution at PAMO-SFP (Physique Atomique, Moleculaire, Optique de la Societe Francaise de Physique) 2016, Bordeaux, $4^{th}$- $7^{th}$ July 2016

C. M. Coppola
"Molecular excitation in hydrogen storage"
Poster contribution at Workshop on Materials Science for Energy Storage, ICTP, Trieste, $11^{th}$-$15^{th}$ May 2015

A. Damone, A. Panarese, C. M. Coppola, J. Jansky, C. Coletti, L. Chiodo, G. Serianni, V. Antoni and S. Longo
"Ab initio modeling of Cs-Mo interfaces in negative ion sources"
Poster contribution, $32^{nd}$ ICPIG, Iasi, Romania, $26^{th}$-$31^{st}$ July 2015

A.Damone, C. M. Coppola, J. Jansky, A. Panarese, G. Serianni, V. Antoni, S.Longo
"Molecular Dynamics of Plasma-Wall Materials for Fusion Technology"
Poster contribution, $31^{st}$ ICPIG, Granada, Spain, $14^{th}$-$19^{th}$ July 2013, Topic number 3

D. Bruno, C. M. Coppola, D. Galli, S. Longo, G. Mizzi, F. Palla
"State-to-state vibrational kinetics of hydrogen plasmas for astrophysical applications"
Poster contribution, $31^{st}$ ICPIG, Granada, Spain, $14^{th}$-$19^{th}$ July 2013, Topic number 7

C. M. Coppola
"State-to-State Vibrational Kinetics of Hydrogen Plasmas in Early Universe Chemistry and Primordial Shock Waves"
Poster contribution, "Mind the gap: from microphysics to large-scale structure in the Universe", 2013, Institute for Astronomy, Cambridge, $8^{th}$-$12^{th}$ July 2013

S. Longo, R. D'Introno, A. Panarese, C.M. Coppola, J. Tennyson
"o-$H_2$, p-$H_2$ and HD vibrational kinetics in the Early Universe"
The Molecular Universe, Posters from the proceedings of the 280th Symposium of the International Astronomical Union held in Toledo, Spain, May 30-June 3, 2011, #240

C. M. Coppola, S. Longo, M. Capitelli, F. Palla, D. Galli
"Vibrational level population of $H_2$ and $H_2^+$ in the early Universe"
The Molecular Universe, Posters from the proceedings of the 280th Symposium of the International Astronomical Union held in Toledo, Spain, May 30-June 3, 2011, #133

C. M. Coppola, P. Diomede, S. Longo
"$H_2(v)$, HD(v) and $H_2^+(v)$ photodissociation rate coefficients in the primordial Universe: thermal contribution"
NOVICosmo, SISSA, Trieste, $20^{th}$-$22^{nd}$ October 2008

C. M. Coppola, P. Diomede, S. Longo
"Parametric calculation of the rate coefficient for the dissociative attachment of $H_2(v)$ for different $T_e$ and $T_v$"
The Molecular Universe, An International Meeting on the Physics and Chemistry of the Interstellar Medium, Arcachon, France, $3^{rd}$-$5^{th}$ May 2008

C. M. Coppola, J. Jansky
"Classical molecular dynamics: simulation of the diffusion of hydrogen atoms on iron surface"
$2^{nd}$ IDEA League Summer School on Multiscale Modelling in Materials Science and Engineering, Simonskall, Germany, $23^{rd}$-$28^{th}$ July 2007

**Teaching**

(Since May 2012) Assistant lecturer in:
"Chemistry"
"Kinetics theory of transport"

**Supervised bachelor thesis**

Loreta Minutilli, September 2017
Antonello Pellecchia, July 2017

**Co-supervised bachelor thesis**

Giuseppe Diana, September 2016 (reading committee)
Tomas Scagliarini, July 2015
Stefano Fiore, April 2015
Francesco Grieco, December 2014
Roberto D'Introno, March 2011

**Supervised master thesis**

Giovanni Mizzi, March 2013

**Other Research Positions**

"Processi elementari e cinetica plasmo-chimica in scariche di idrogeno"
University of Bari, $7^{th}$ August 2010 – $1^{st}$ Marzo 2011

"Montecarlo models for non-equilibrium gases and plasmas"
University of Bari, $24^{th}$ September 2007 – $30^{th}$ January 2008

"Software for $H_2$ plasma modeling in Cosmology"
CNR-IMIP Bari, $29^{th}$ March 2007 – $1^{st}$ June 2007

"Development of neutral and ionized reactive fluxes and their interaction with surfaces"
University of Bari, $24^{th}$ January 2007 – $30^{th}$ May 2007

**Awards & Projects**

Galileo 2018
Italian PI for the funded project "HD chemistry in the early Universe (formation, excitation and destruction)" with Université du Havre, Le Havre (FR) (4,411 Euro for the Italian side)

PI for the ESA project: "Challenges related to the design of a reservoir for the transport of $H_2$" (200,000 Euro)

COST STSM Reference Number: COST-STSM-CM1401-32961
STSM Topic: H + HD / D + H2 collisions and new H + H2/HD collisional cooling

function (part I)
Host: Francois Lique, Université du Havre, Le Havre (FR), March 2016

Principal investigation of the project 'MESH: Molecular excitation in storage of hydrogen' funded for the call "Future in Research 2014". The budget allocated for this position is $\sim$ 105,000 Euro.

Team leader of the international group "EUROPA - Early Universe: Research On Plasma Astrochemistry" at International Space Sciences Institute - Bern (Switzerland). The group is constituted by scientists from worldwide institutions: USA, UK, Japan, Sweden, France, Germany, Chile, Italy. The budget allocated for each international group is $\sim$ 16,000 Euro.

Regional winner for the project "Bollenti Spiriti", 2007-2010

National Math Olympiad Finalist "Campionati Internazionali di giochi matematici", Centro PRISTEM, Università Bocconi, 2000

**Languages and Technologies**

Good knowledge of Linux. Basic Windows and MacOS user (I strongly support open source projects and free software policy).
Fluent in Fortran (up to the most recent standard - Fortran 2008) along with the usage of the following libraries: Numerical Recipes, GNU Scientific Library. PBS job scheduler. Version control system: git. Good knowledge of: Latex, Python (together with iPython and Jupyter; libraries: NumPy, SciPy, Matplotlib, Pandas, Astropy), Linux Shell Programming - bash, OpenOffice. Familiar with: MATLAB, HTML, Mathematica. Basic knowledge of C++, Java

**Certificates**

1. Neural Networks and Deep Learning by deeplearning.ai on Coursera. Certificate earned on October 5, 2017. Grade Achieved: 96.4%
2. Introduction to Data Science in Python by University of Michigan on Coursera. Certificate earned on January 5, 2017. Grade Achieved: 92.3%

**Research Interests**

My research interests include modeling chemical systems from very large (Hubble radius, i.e. approximately the dimension of our Universe) down to small (few Böhr radii) scales; in particular, I have developed simulations in early Universe chemistry, state-to-state chemical kinetics, non-equilibrium phenomena in plasmas, quantum chemistry, collisional-radiative models and molecular dynamics.

Theoretical physics and chemistry have been the main research topics of pre-graduate and doctoral courses; numerical simulations have been used as predominat tool in this investigation. After the General Relativity examination I was invited by Prof. Maurizio Gasperini to do my bachelor thesis in Physics with him on string theory. In particular, I focused on the motion of a bosonic string and some introductory aspects to its quantization and I simulated its motion using Mathematica. After that, I moved to study plasma physics for the master thesis in Theoretical Physics. In particular, I studied the relevance of the inclusion of the excited levels of $H_2$ in the evaluation of reaction rates for some processes that are important in the early Universe chemistry. Both LTE and non-equilibrium level populations have been used in the calculation of some rate coefficients for chemical processes involving $H_2$ and $H_2^+$; the comparison has shown that important differences arise especially at low redshift $z$.

During the period of my PhD in Chemical Sciences I developed a state-to-state time dependent kinetics for $H_2$ and $H_2^+$ in gas phase conditions for the early Universe chemistry. This research introduced me to a personal interest in modeling non-equilibrium phenomena. So far in my research activity, this topic has been studied concerning the molecular vibrational distribution functions and distortion photons due to molecular radiative cascade in the early Universe context. I spent part of my PhD in the Arcetri Astrophysical Observatory, under the supervision of proff. Daniele Galli and Francesco Palla.

As a honorary research associate I have worked for one year at UCL-Physics & Astronomy Department supervised by Prof. Jonathan Tennyson; eventually, I focused on quantum chemistry, in particular on the evaluation of linelist for molecules relevant in the early Universe chemistry and on calculation of cooling functions.

The study of early Universe chemistry was instrumental in deepening my knowledge of chemical processes occurring in gas phase and involving mainly $H_2$ and its deutereted variant HD.

During the first year of my PhD I have also developed a classical molecular dynamics simulation for the formation of $H_2$ on iron samples and calculated the diffusion coefficient. This simulation has been mutuated and recently applied to the system Mo/Cs for fusion technology applications.

In the last year I have developed an increasing personal interest on hydrogen economy and storage; I have realized that this topic has an important role not only in the everyday life of people but it is fundamental also on large scale transportation, as in the case of aerospace. My project consists in the analysis and simulation via molecular dynamics of several materials suitable to store hydrogen; in particular, the role of molecular excitation will be investigated.

**Other interests**

Piano intermediate diploma at Conservatorio di musica- Vicenza
I have studied harpsichord with Prof. Giulia Nuti (Fiesole - Florence) and I playes in a Renaissance/Baroque ensemble called "*L*a recercada"

**Conferences/ Schools Attended**

"The Astrochemical week",
Faro, 17-19 January 2017

"Hydride Toolbox",
Paris, Universite Pierre et Marie Curie, 12-15 December 2016

"International Meeting on Atomic and Molecular Physics and Chemistry 2016",
Universit du Havre, 27-30 June 2016

"Corso intensivo di programmazione di schede grafiche utilizzando CUDA",
Dipartimento di Fisica e Sezione INFN di Bari, 11-13 May 2016

"High Performance Molecular Dynamics",
CINECA, Casalecchio di Reno (Bo), 18-20 November 2015

"COST Action Our Astrochemical History CM1401, First General Meeting in Prague",
Prague (Czech Republic), 25-29 May, 2015

"Workshop on Materials Science for Energy Storage",
Trieste ICTP, 11-15 May 2015

"Leiden Observatory workshop: Photodissociation in astrochemistry",
Leiden (The Netherlands), 35 February 2015

"III Workshop on Active Galactic Nuclei and Gravitational Lensing",
Končarevo (Serbia), 7-11 October 2014

"23rd Summer School on Parallel Computing", CINECA, Segrate (Mi), 8-19 September 2014

"Bilbao Quantum Days: Mathematical Methods in Atomic and Molecular Physics", BCAM, Bilbao, July 15-16, 2014

"$41^{st}$ EPS Conference on Plasma Physics", Berlin, 23-27 June 2014

"Introduction to Fortran90", CINECA, Casalecchio di Reno (Bo), 21-24 October 2013

"Mind the gap: from microphysics to large-scale structure in the Universe", 2013, Institute for Astronomy, Cambridge, 8-12 July 2013

"The low-metallicity ISM: Chemistry, turbulence and magnetic fields", Georg-August-Universität, Göttingen, 8-13 October 2012

"Theoretical and computational astrochemistry", Arcetri, 30 - 1 September 2012

"EWASS 2012", Rome, 1 - 4 July 2012

"Data and models for the chemistry of the early Universe", Arcetri, 6 - 7 February 2012

"The chemical Cosmos, Annual Conference", Malta, 12  14 October 2011

"The Molecular Universe: 280 IAU Symposium", Toledo, May 30 - June 3, 2011

"Workshop Astrochemistry: Molecular Networks connecting the Universe", Amster-

dam, 18 - 20 April 2011

"Molecole nello spazio e nel tempo", Accademia Lincei, Roma, 4-5 November 2010

"IUPAC 2009", Glasgow, Scotlad, 2-7 August 2009

"Novicosmo 2008", SISSA, Trieste, Italy, 20-22 October 2008

"The molecular Universe: an International meeting on Chemistry and Physics of the Interstellar medium", Arcachon, France, 5-8 May 2008

"Physics and technology Plasma-enhanced PVD methods", Bad Honnef Physiczentrum, Germany, 11-13 October 2007

"Low Temperature Plasma Physics: Basics and Application", Bad Honnef Physiczentrum, Germany, 6-11 October 2007

"Multiscale Modelling in Materials Science and Engeneering", Eifel Mountains, Germany, 22-28 July 2007

"$41^{st}$ Course: Molecular Physics and Plasmas in Hypersonics", Ettore Majorana foundation and centre for scientific culture, Erice, 01-07 August 2005

"The Physics of LHC: theoretical tools and experimental challenges, 9 - 14 June 2005

**Science Community Service**

1. Referee experience for
   - Astronomy & Astrophysics;
   - Journal of Astronomy and Astrophysics;
   - The Astrophysical Journal
2. Leader of the team "EUROPA - Early Universe: Research On Plasma Astrochemistry" at International Space Science Institute (Bern)
   This project has been approved by ISSI in 2013 and it focused on the chemistry of early Universe and on the birth of the first structures in our Universe. For more details on the topics and on the participants please visit our website:
   `<http://www.issibern.ch/teams/europa/EUROPA.html>`
3. Scientific committee member of the conference "International Meeting on Atomic and Molecular Physics and Chemistry" 2016