



## **OBSERVATORY FOR ASTROCHEMICAL KINETICS AND RELATED ASPECTS**

**June 27<sup>th</sup> and 28<sup>th</sup>, 2019**

*Library of the Accademia Nazionale delle Scienze, detta dei XL  
Scuderie Vecchie, Villa Torlonia, Via L. Spallanzani 1/A*

**In collaboration with Accademia Nazionale dei Lincei, Università di Perugia**

*Celebrating 160 years from Arrhenius birthday and 130 years of remarkable success of his equation, open problems on its foundations and perspectives of future applications are under focus.*

Astrochemistry, a highly interdisciplinary research area, relies on Earth-based diffuse “observatories” on nature, structure and transformations of molecular Universe: detected molecules, identified from spectroscopic and radio-astronomical observations, space-mission data collections, laboratory experiments, computational modeling, are continuously increasing in number, leading to decisive progress into the understanding of the chemical evolution from the early formation of atomic, molecular, radical, ionic species. The stepping stones require consolidation by concerted chemical kinetics and molecular dynamics: the meeting aims at connecting experimental and theoretical knowledge by (i) coordinating groups of spectroscopists, astrophysicists, quantum chemists to interact with chemical kineticists within a decade-old established network “Astrochemical Observatory”; (ii) indicating molecular-beam experiments to characterize dynamical and kinetic properties involving interstellar molecules; (iii) assessing role of molecular orientation in chiral discrimination processes, arguably occurring in primordial environments; (iv) developing theoretical models for reactive processes— important those involved in chirality-selective processes and in low-temperature manifestations of non-Arrhenius behavior. Enrichment of current reaction-rate databases is crucial; tessellation of an immensely wide mosaic, with few sparse pieces known, opens mankind to an arguably infinite search: indeed, there is no certainty that these experimental measurements and theoretical approaches will provide the photodynamical or collisional mechanisms that for example played a role in a prebiotic context for the natural emergency of selective chirality: yet, it is an educated guess that they will lead to progress, extending instrumentation and simulation techniques of molecular science in a joint effort of Italian groups with teams already called to collaborate.



## PROGRAMME

### Thursday 27 June

14.00 – 14.15: Presentation, Annibale Mottana (President Accademia Nazionale delle Scienze, detta dei XL)

*Chair: Vincenzo Aquilanti*

14.15 – 14.50: Roger Anderson (University of California – Santa Cruz, USA): *Discrete wavefunction Description of Time Evolution in Uni-molecular Photo Processes*

14.50 – 15.25: Constantino Tsallis (Centro Brasileiro de Pesquisas Físicas, Brazil): *Applications of nonadditive entropies in natural, artificial and social complex systems*

15.25 – 15.45: Lorenzo Avaldi (CNR Roma): *On the mechanisms of formation and decomposition of peptide bonds*

15.45 – 16.05: Walther Caminati (Università di Bologna): *Information on Chemical Kinetics from Rotational Spectroscopy*

16.05 – 16.25: Antonio Laganà (Università di Perugia): *Open molecular science cloud services for astrochemical processes*

16.25 – 16.45: Fernando Pirani (Università di Perugia): *New insights on the Stereodynamics of elementary processes*

16.45 – 17.05: Maria Rutigliano (CNR Bari): *Rotational Inelastic Scattering of H<sub>2</sub> and O<sub>2</sub> Molecules from Graphite*

17.05 – 17.25: Annarita Laricchiuta (CNR Bari): *CO molecule excitation and ionization by electrons/ H H<sup>+</sup> resonant charge exchange in dense plasmas*

17.25 – 18.00: Ernesto Borges (Universidade Federal da Bahia, Brazil): *Non-Boltzmann distributions in small bodies of the Solar System*

18.00 – 18.35: José Cernicharo (Madrid): TBA

### Friday 28 June.

*Chair: Federico Palazzetti*

9:00 – 9:35: Cecilia Ceccarelli (Université de Grenoble-Alpes, France): *Astronomical observations as tools to test and constrain quantum chemistry calculations of interstellar organic chemistry*

9.35 – 9.55: Carlo Petrongolo (CNR Pisa): *NonAdiabatic Quantum Astrochemistry: Kr+OH\* Electronic Quenching*

9.55 – 10:15: Dario De Fazio (CNR Roma): *The role of the Helium chemistry in the early universe evolution: a rigorous quantum mechanical approach*

10.15 – 10.35: Fabrizio Esposito (CNR Bari): *Back to QCT and beyond*

10.35 – 10.55: Claudio Codella (INAF, Firenze): *Astrochemistry at work around Sun-like star forming regions: from protostars to planets*

10.55 – 11.15: Pier Luigi Gentili (Università di Perugia): *Astrochemistry and the theory of Complex Systems*



11.15 – 11.35: Coffee Break

*Chair: Mario Capitelli*

11.35 – 11.55: Susanna Piccirillo (Università di Roma Tor Vergata): *Ultra-Fast -VUV Photoemission Study of UV Excited 2-Nitrophenol*

11.55 – 12.15: Stefano Turchini (CNR Roma): *Fast Transient Absorption and Time-Resolved Photoelectron Spectroscopy of Optically Excited Molecules*

12.15 – 12.35: Luca Evangelisti (Università di Bologna): *Kinetics and thermodynamics in reactions studied by microwave spectroscopy*

12.35 – 12.55: Gianpiero Colonna (CNR Bari): *Hypersonic entry in giant planets: self-consistent state-to-state approach*

12.55 – 13.15: Daniela Pietanza (CNR Bari): *Self-consistent Electron and Vibrational Energy Distribution Functions in Microwave CO<sub>2</sub> plasmas*

13.15 – 14.00: Lunch

*Chair: Andrea Lombardi*

14.00 – 14.20: Savino Longo (Università di Bari): *Deterministic models of gas-surface kinetics based on the formalism of radiative transfer*

14.20 – 14.40: Domenico Giordano (ESA-ESTEC, The Netherlands): *Considerations regarding the Schrödinger-equation separability with application to the one-dimensional hydrogen atom*

14.40 – 15.00: Gaia Micca Longo (Università di Bari): *Quantum confinement as a model for hydrogen species under extreme conditions*

15.00 – 15.20: Noelia Fagnas Lago and Marzio Rosi (Università di Perugia): *Interstellar dimethyl ether gas-phase formation: a quantum chemistry and kinetics study*

15.20 – 15.30: Nadia Balucani (Università di Perugia): *Chemical parenthood in space*

15.30 – 15.40: Demian Marchione (Università di Perugia): *An experimental study of the pyridine (C<sub>5</sub>H<sub>5</sub>N) + O atom reaction: gas-phase destruction routes of a long searched molecule in extra-terrestrial environments.*

15.40 – 16.00: Danilo Calderini (ETH Zurich): *Quantum tunneling and the geometric-phase effect*

16.00 – 16.20: Olga De Pascale (CNR Bari): *Carbon detection by laser induced breakdown spectroscopy in meteorites*

16.20 – 16.40: Vincenzo Laporta (CNR Bari): *Electron-molecule dynamics for non-equilibrium plasmas.*

16.40 – 16.50: Conclusions

SCIENTIFIC AND ORGANIZING COMMITTEE

***Vincenzo Aquilanti, Andrea Lombardi and Federico Palazzetti***

**Please confirm your participation to [segreteria@accademixl.it](mailto:segreteria@accademixl.it)**