



Southern European Conference on the Science of Molecules
Perugia, 27-29 September 2023

Program of the conference

Day 1, 27/09/2023 (ROOM G)

9:40 Registration/Opening

SESSION 1 - Chairperson: **ANDREA LOMBARDI**

10:00 [O1] **TOMÁS GONZALEZ LEZANA**

Atom-diatom complex forming reactions and ordered solvation shells in doped helium clusters

10:30 [O2] **CECILIA COLETTI**

The many faces of vibrational relaxation dynamics in N₂-O collisions

11:00 Coffee break

SESSION 2 - Chairperson: **NOELIA FAGINAS LAGO**

11:30 [O3] **MARKO CVITAŠ**

Tunnelling splittings of rovibrationally excited states of molecules via the semiclassical instanton theory

12:00 –12:30 [O4] **LORIANO STORCHI**

Machine and Deep Learning techniques in chemistry: from DeepGRID to a simple formula generator

13:00 Lunch at “Teatro Morlacchi”

SESSION 3 - Chairperson: **CECILIA COLETTI**

15:00 [O5] **ANDREA LOMBARDI**

Preliminary assessment of C₆₀ as a reaction site for space chemistry

15:30 [O6] **JENNIFER NOBLE**

Vibronic spectroscopy as a probe of structure and dynamics in aromatic molecules

16:00 Coffee break

SESSION 4 - Chairperson: **TOMÁS GONZALEZ LEZANA**

16:30 [O7] **JORGE MARQUES**

Modeling microsolvation of ions: achievements and future perspectives



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17:00 [O8] **GIACOMO GIORGI**
*Tailoring High-Entropy Oxides as Emerging Radiative Materials
for Daytime Passive Cooling*

Day 2, 28/09/2023 (ROOM B)

SESSION 5 - Chairperson: **JORGE MARQUES**

9:30 [O9] **GIOVANNI BISTONI**
*Combining high accuracy and chemical insight with local coupled
cluster methods*

10:00 [O10] **PASCAL LARREGARAY**
Energy Transfers upon Hydrogen Atom Scattering off Tungsten Surfaces

10:30 [O11] **NOELIA FAGINAS LAGO**
*Coding Cross Sections of an Electron Charge Transfer Process: Analysis
of Different Cuts for the Entrance and Exit Potentials*

11:00 Coffee break

SESSION 6 - Chairperson: **PASCAL LARREGARAY**

11:30 [O12] **JOSÉ D. GOUVEIA**
*Effect of surface functionalization on the adsorption of small molecules by
the titanium carbide mxene*

12:00 – 12:30 [O13] **MASSIMILIANO BARTOLOMEI**
*Molecular sieving and adsorption by exploiting 2D membranes based on
gamma-graphynes*

13:00 Lunch at “Teatro Morlacchi”

15:00 Panel discussion: building a SECSMol community, what’s next?

16:00 Coffee break

18:30 Excursion and social aperitif

20:00 Social Dinner



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Day 3, 29/09/2023 (ROOM G)

SESSION 7 - Chairperson: **MARKO CVITAŠ**

10:00 [O14] **REGIS BISSON** (from remote)

Molecules, radicals and molecular ions in interaction with surfaces: interests for nuclear fusion

10:30 [O15] **GABRIELLA DI GENOVA**

Rate coefficient for the formation of AIO by radiative association

11:00 Coffee break

SESSION 8 - Chairperson: **LORIANO STORCHI**

11:30 [O16] **MARZIO ROSI**

A computational study of the reaction between N(2D) and simple aromatic hydrocarbons

12:00 [O17] **LUCA MANCINI**

A Theoretical characterization of bimolecular reactions leading to the formation of Interstellar phosphorous and silicon-bearing molecules

12:30 Concluding remarks

13:00 Lunch at "Teatro Morlacchi"