



4-5 APRIL 2019

YOUNG RESEARCHERS MEET MOLECULAR SPECTROSCOPY

Sala Stemmi
Palazzo della Carovana
Scuola Normale Superiore
Piazza dei Cavalieri, 7 - Pisa

INVITED SPEAKERS

ALBERTO BAIARDI
ETH Zurich

LUCA EVANGELISTI
University of Bologna

IKER LEÓN
University of Valladolid

DANIELE LICARI
Istituto Italiano di Tecnologia

VINCENT LIÉGEOIS
University of Namur

CHRISTIAN MERTEN
Ruhr-University Bochum

HA VINH LAM NGUYEN
LISA - Paris

ALFONSO PEDONE
University of Modena and Reggio Emilia

Elaborazione a cura del Servizio Comunicazione e Relazioni Esterne | SNS

Info
<http://smart.sns.it/yrms2019/>

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NORMALE
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SCIENTIFIC COMMITTEE

JULIEN BLOINO

Scuola Normale Superiore

WALTHER CAMINATI

University of Bologna

JENS-UWE GRABOW

Leibniz University Hannover

CRISTINA PUZZARINI

University of Bologna

SERGIO RAMPINO

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LORENZO SPADA

Scuola Normale Superiore

MONICA SANNA

Scuola Normale Superiore

JACOPO BALDINI

Scuola Normale Superiore

The goal of this conference is to provide a platform to exchange ideas and promote collaborations within the community of young computational and experimental researchers (especially PhD students, Post-Docs, Assistant Professors) who have already provided significant contributions to the broad field of molecular spectroscopy.

This event is especially intended for the next generation of spectroscopists who are the “future” in using, developing and advancing the new tools and instruments becoming available nowadays thanks to new technological advancements (cutting-edge experimental spectroscopic instruments, state-of-the-art computational techniques, new-frontier land-based, air- and space-borne telescopes, intelligent data analysis).

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SESSION III

08:50 Registration and Welcome

09:25 Opening

SESSION I

Session chair, JULIEN BLOINO

09:30 CHRISTIAN MERTEN, Ruhr-University Bochum
Matrix-isolation VCD spectroscopy: Towards the characterization of chiral reactive intermediates

10:00 QIN YANG, Scuola Normale Superiore
Theoretical Investigations of the Optical Properties of Helicene-Iridium Complexes

10:20 MARCO FUSÈ, Scuola Normale Superiore
Chiral properties of transition metal complexes: computational approaches

10:40 MARTIN PIŽL, Czech Academy of Sciences
Time-resolved vibrational spectra of Ru and Re diimine complexes: Anharmonic calculations

11:00 Coffee Break

SESSION II

Session chair, NICOLA TASINATO

11:20 VINCENT LIÉGEOIS, University of Namur
New tools to unravel the vibrational signatures of molecules - Application to Raman optical activity and to sum-frequency generation signatures

11:50 FUCSIA CREA, Freie Universität Berlin
Photo-activation of mechanosensitive ion channels

12:10 MATTIA SAITA, Freie Universität Berlin
Giving shape to protonated water clusters in membrane proteins with polarized FTIR

12:30 SANDRA MÓNICA VIEIRA PINTO, Scuola Normale Superiore
In silico Infrared Spectroscopy of Protein Side Chains

12:50 Lunch

14:20 MARCO MENDOLICCHIO, Scuola Normale Superiore
Anharmonic vibrational treatment of linear, symmetric and asymmetric molecules

Session chair, WALTHER CAMINATI

14:40 LUCA EVANGELISTI, University of Bologna
Challenges in Microwave Spectroscopy

15:10 THUY NGUYEN, LISA - Paris
Microwave spectroscopic and quantum chemical investigations on 2-methylpyrrole

15:30 SILVIA ALESSANDRINI, Scuola Normale Superiore
Benchmark of quantum-chemical computations for molecules containing second-row atoms

15:50 HA VINH LAM NGUYEN, LISA - Paris
Understanding (Coupled) large amplitude motions: The interplay of microwave spectroscopy, spectral modeling, and quantum chemistry

16:20 MARIE-LUISE HEBESTREIT, Heinrich-Heine-University - Düsseldorf
Position dependent study on 3-, 4-, and 5-Cyanoindole via high resolution laser induced Stark spectroscopy

16:40 Coffee Break

SESSION IV

Session chair, SERGIO RAMPINO

17:00 DANIELE LICARI, Istituto Italiano di Tecnologia
Latest developments in VMS Draw

17:30 SURAJIT NANDI, Scuola Normale Superiore
A Modern-Fortran Program for Chemical Kinetics on top of Anharmonic Vibrational Calculations

17:50 JACOPO LUPI, Scuola Normale Superiore
Quantum mechanical strategies for reactivity and kinetics of atmospheric reaction pathways

18:10 BALASUBRAMANIAN CHANDRAMOULI, Scuola Normale Superiore
Examining molecular conformational landscape using QM based stochastic approach

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SESSION V

Session chair, JENS-UWE GRABOW

- 9:00 ALBERTO BAIARDI, ETH Zurich
Efficient quantum dynamics with the Time-Dependent Density Matrix Renormalization Group
- 9:30 MATTHEW TURNER, University of Warwick
Identifying Secondary Species in Solution: A Combined Experimental and Theoretical Approach
- 9:50 IKER LEÓN, University of Valladolid
Molecular Spectroscopy: A Collaborative Effort
- 10:20 DRAGOS LUCIAN ISAC, Petru Poni Institute of Macromolecular Chemistry - Iasi
Computational determination of the charge transfer excited state in azobenzene maleimide derivatives
- 10:40 SARA DEL GALDO, Scuola Normale Superiore
An effective integration of variational and perturbative QM/MM approaches for computing UV-Vis spectra in condensed phases
- 11:00 Coffee Break

SESSION VI

Session chair, LORENZO SPADA

- 11:20 ALFONSO PEDONE, University of Modena and Reggio Emilia
Computational solid-state NMR spectroscopy as a tool for the structure determination of oxide glasses and assessment of classical Force-Fields
- 11:50 FEDERICA ROSSI, University of Torino
The accurate ^1H - ^{14}N distance measurement by phase-modulated RESPDOR at ultra-fast MAS
- 12:10 SIMONE BORDIGNON, University of Torino
2D solid-state NMR experiments to characterize the hydrogen bond network in pharmaceutical cocrystals
- 12:30 SILVIA HRISTOVA, Bulgarian Academy of Sciences
 β -diketones based rotary switches: molecular spectroscopy and computational chemistry playing together
- 12:50 Closing and lunch

Name Surname	Institution	Country
Roy Aerts	University of Antwerp	Belgium
Silvia Alessandrini	Scuola Normale Superiore	Italy
Alberto Baiardi	ETH Zurich	Switzerland
Jacopo Baldini	Scuola Normale Superiore	Italy
Akash Deep Biswas	Scuola Normale Superiore	Italy
Julien Bloino	Scuola Normale Superiore	Italy
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Luca Evangelisti	University of Bologna	Italy
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Marco Fusè	Scuola Normale Superiore	Italy
Jens-Uwe Grabow	Leibniz University Hannover	Germany
Marie-Luise Hebestreit	Heinrich-Heine-University Düsseldorf	Germany
Silvia Hristova	Bulgarian Academy of Sciences	Bulgaria
Dragos Lucian Isac	"Petru Poni" Institute of Macromolecular Chemistry	Romania
Iker León	Universidad de Valladolid	Italy
Daniele Licari	Istituto Italiano di Tecnologia (IIT)	Italy
Vincent Liégeois	University of Namur	Belgium
Jacopo Lupi	Scuola Normale Superiore	Italy
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Mattia Melosso	University of Bologna	Italy
Marco Mendolicchio	Scuola Normale Superiore	Italy
Christian Merten	Ruhr-University Bochum	Germany
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Ha Vinh Lam Nguyen	Laboratoire LISA	France
Thuy Nguyen	Laboratoire LISA	France
Alfonso Pedone	University of Modena and Reggio Emilia	Italy
Martin Pižl	J. Heyrovský Institute of Physical Chemistry of the CAS	Czech Republic
Cristina Puzzarini	University of Bologna	Italy
Sergio Rampino	Scuola Normale Superiore	Italy
Federica Rossi	University of Torino	Italy
Laura Rotundo	University of Torino	Italy
Mattia Saita	Freie Universität Berlin	Germany
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Lorenzo Spada	Scuola Normale Superiore	Italy
Nicola Tasinato	Scuola Normale Superiore	Italy
Matthew Turner	University of Warwick	United Kingdom
Tom Vermeyen	University of Antwerp	Belgium
Sandra Mónica Vieira Pinto	Scuola Normale Superiore	Italy
Qin Yang	Scuola Normale Superiore	Italy
Jiang Zhongming	Scuola Normale Superiore	Italy



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