



UNIVERSITÀ  
DEGLI STUDI  
DI BRESCIA

BRESCIA  
2018



6<sup>th</sup> International Conference on  
Vibrational Optical Activity



Brescia, Italy  
September 9<sup>th</sup>/13<sup>th</sup>, 2018

**FINAL PROGRAMME**

## INTERNATIONAL STEERING COMMITTEE

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**Hua-Jie (Jack) Zhu** - China

## LOCAL ORGANIZING COMMITTEE

**Sergio Abbate**

Giovanna Longhi

Giuseppe Mazzeo

Ivano Alessandri

Simone Ghidinelli

Ernesto Santoro

*(Università degli Studi di Brescia)*

**Vincenzo Barone**

Lorenzo Paoloni

Nicola Tasinato

Monica Sanna

*(Scuola Normale Superiore, Pisa)*

## *Welcome to Brescia!*

On behalf of the local organizing committee, we welcome you at the sixth installment of the VOA conference series. As in the previous version of the series, the main focus of this meeting is to present the cutting edge in vibrational optical activity (VOA), highlighting the newest research developments in the field, both experimentally and theoretically. In addition to the newest progress in vibrational circular dichroism (VCD) and Raman optical activity (ROA), and in continuity with the previous edition, this year's program will also host some latest developments of neighboring fields, CPL (circularly polarized luminescence), MCD (magnetic circular dichroism) and superchiral field spectroscopy. Most importantly, the conference will contain two sessions on Astrochemistry, dealing with the investigation and (possible) spectroscopic detection of chiral molecules in the Universe. The meeting offers a total of 56 lectures, divided out on 23 invited talks and 33 oral contributions. One of the invited talks will be the opening lecture, rewarding the best journal paper in the field of VOA in the last two years, in honor of the late Philip J. Stephens. We are happy to announce that some of the invited talks and oral contributions will be presented by young scientists, at the beginning of their scientific life. In addition to the oral program 22 (and counting) poster presentations will conclude the scientific offerings of VOA-6. We hope that the all the conferees will enjoy the program, and, most importantly, will take the opportunity to exchange ideas and projects, and establish new collaborations.

To make the participants appreciate the history and atmosphere of Brescia, which has been an old Celtic, Roman and Lombard city, a guided tour of the City Museum of Santa Giulia will be offered to all participants. Santa Giulia is an old convent hosting ruins from the first century A.D.; in this convent Irmgaard, the repudiated wife of Charle Magne, spent her last days as a nun, and nowadays it hosts masterpieces from Middle Ages to Renaissance.

Finally we are pleased and grateful from the contributions of our sponsors, whose support has been vital for keeping the registration fees at the same level of the previous edition, and for allowing the programme being offered.

Sergio Abbate and Vincenzo Barone, Conference Chairs.

## STEPHENS AWARD

The Philip J. Stephens Award was established in 2014 by the International Steering Committee of Vibrational Optical Activity (VOA) at the VOA-4 meeting in Baoding, China. The award was presented for the first time at the VOA-5 conference in Antwerp, Belgium in 2016 and honors Philip J. Stephens (West Bromwich, UK, 10/9, 1940 – Los Angeles, CA, 7/31, 2012) as one of the leading founders of the VOA field with particular influence on vibrational circular dichroism (VCD) measurement and theory.

In order to distinguish this award from those in more established fields, and to place greater emphasis on encouraging the creative development of VOA as a field, the award is presented at each VOA conference to the authors of the paper judged to be most deserving published in the two calendar years prior to the conference.

The designated author of the paper presents the Philip J. Stephens Award Address at the VOA conference. All authors of the award will receive a framed certificate commemorating the award. The International Steering Committee considers all papers published on VCD and ROA in the two years prior to each VOA conference, without any nomination process, and votes for an award selection. In VOA-5 the paper was: "A novel Raman optical activity instrument operating in the deep ultraviolet spectral region" by Josef Kapitán; Laurence D. Barron; Lutz Hecht, *Journal of Raman Spectroscopy* (2015), 46(4), 392-399, presented by Josef Kapitán, Palacký University Olomouc, Czech Republic.

The winning paper for VOA-6 is: "Effective Fully Polarizable QM/MM Approach To Model Vibrational Circular Dichroism Spectra of Systems in Aqueous Solution" by Tommaso Giovannini; Marta Olszowka; Chiara Cappelli, *Journal of Chemical Theory and Computation* (2016), 12(11), 5483-5492. The paper (and further developments) will be presented by Chiara Cappelli, Scuola Normale Superiore, Pisa, Italy.

SUNDAY September 9<sup>th</sup>

- 03.30 pm      **Secretariat Desk Opening & Participants' Registration**
- 05.00 pm      **Opening Ceremony and Welcome Address**  
Maurizio Tira  
*Rector University of Brescia*  
Vincenzo Barone  
*Chairman of Scuola Normale Superiore Pisa and Conference Chairman*  
Silvano Sozzani  
*Chairman of Molecular and Translational Medicine Dept, University of Brescia*  
Sergio Abbate  
*University of Brescia, Conference Chairman*
- 05.15 pm      **STEPHENS AWARD PRESENTATION & AWARD ADDRESS**  
**IS 1**  
**Effective fully polarizable QM/MM approach to model vibrational circular dichroism spectra of systems in aqueous solution**  
Chiara Cappelli (Italy)
- 06.00 pm      **Welcome Cocktail**

## MONDAY September 10th

08.30 am **Secretariat Desk Opening**

### *I SESSION "PAST, PRESENT and FUTURE of VOA"*

09.00 am **IS 2**

**45 years of vibrational optical activity**

Prasad L. Polavarapu (USA)

09.45 am **IS 3**

**Variability of VOA Theory and Experiment**

Petr Bouř (Czech Republic)

10.30 am *coffee break*

### *II SESSION "VCD&ROA EXPERIMENTAL"*

11.00 am **IS 4**

**VCD studies on matrix-isolated molecule**

Corina Pollok (Germany)

11.30 am **O IDN 25**

**A Spectroscopic Ruler for Measuring Active Site Distortions based on Raman Optical Activity of a Hydrogen Out-of-Plane Vibration**

Masashi Unno (Japan)

11.50 am **O IDN 56**

**Biofluid Analysis – A challenge to chiroptical spectroscopy**

Lucie Harbatová (Czech Republic)

12.10 pm **O IDN 74**

**Molecular structure analysis of pantolactone using chiroptical spectroscopies**

Jun Koshoubu (Japan)

12.30 pm **O IDN 58**

**Resonance-Induced Enhancement of Solvent Vibrational Raman Optical Activity**

Jiří Kessler (Czech Republic)

12.50 pm *lunch*

### *III SESSION "VCD&ROA Theory and Ab-Initio Calculation"*

01.50 pm **IS 5**

**Accurate vibrational spectra of chiral medium-sized molecules: simulations beyond the harmonic approximation**

Julien Bloino (Italy)

02.20 pm **O IDN 66**

**Complementarity in Chiroptical Spectroscopy: divide and conquer molecular flexibility**

Valentin Paul Nicu (Romania)

02.40 pm **O IDN 38**

**Exploring the combination and overtone vibrations by Raman optical activity**

Pavel Michal (Czech Republic)

- 03.00 pm **O IDN 48**  
**A Partial Spectrum Approach in Infrared Absorption and Vibrational Circular Dichroism**  
T.Q. Teodoro (The Netherlands)
- 03.20 pm **O IDN 51**  
**An efficient technique to calculate vibrational circular dichroism spectrum**  
Chandan Kumar (The Netherlands)
- 03.40 pm **O IDN 75**  
**Problems with interpretation of chiroptical spectra by using quantum chemical calculations**  
Joanna Rode (Poland)
- 04.00 pm *coffee break*
- IV SESSION "VCD&ROA: MD simulations (QM/MM and some address to Aggregation, Band-shape, etc.)"*
- 04.30 pm **IS 6**  
**Calculation of Vibrational Circular Dichroism: Correlations in Space and Time**  
Sascha Jähnigen (Germany)
- 05.00 pm **O IDN 10**  
**Probing molecular chirality, learning about solvation**  
Christian Merten (Germany)
- 05.20 pm **O IDN 60**  
**VOA of Aqueous Solutions: Hydrogen Bonding vs. Conformational Flexibility**  
Tommaso Giovannini (Italy)
- 05.40 pm **O IDN 29**  
**Exploring resonance ROA of bioactive chromophores: ligand binding to a highly ruffled haem moiety**  
Roberta Sgammato (Belgium)
- 06.00 pm **O IDN 39**  
**Astaxanthin aggregates studied by molecular dynamics and electronic circular dichroism spectroscopy**  
Grzegorz Zajac (Poland)
- 06.20 pm **O IDN 45**  
**Explicit solvation of carboxylic acids for vcd studies: limiting the computational efforts without losing accuracy**  
Karoline Bünnemann (Germany)
- 06.40 pm **O IDN 72**  
**Explicitly solvating small molecules with a Monte Carlo approach**  
Matteo Tommasini (Italy)

TUESDAY September 11<sup>th</sup>

08.30 am Secretariat Desk Opening

*VI SESSION "ROA/VCD Experimental Old&New"*

09.00 am

IS 7

Time-domain measurement of the complex chiro-optical susceptibility by an ultra-stable common-path interferometer

Dario Polli (Italy)

09.30 am

IS 8

Resonance Raman Optical Activity of xanthophylls' supramolecular assemblies: homomolecular and mixed systems

Małgorzata Barańska (Poland)

10.00 am

O IDN 47

Spectrometer for measurement of Raman optical activity in the extended spectral range

Josef Kapitán (Czech Republic)

10.20 am

O IDN 64

Resonance Raman optical activity of human serum transferrin

Jonathan Bogaerts (Belgium)

10.40 am

O IDN 15

Histidine complexes with metals studied by multiple spectroscopic methods

Jana Hudecová (Czech Republic)

11.00 am

*coffee break*

*VI SESSION "ROA and non-linear spectroscopies"*

11.30 am

IS 9

High sensitive chiral Discrimination by heterodyne-detected VSGS Spectroscopy

Taka-aki Ishibashi (Japan)

12.00 pm

O IDN 17

Enhancing circular dichroism at the nanoscale

Paolo Biagioni (Italy)

12.20 pm

O IDN 59

Is it Possible to Enhance Vibrational Circular Dichroism Signals with Tailor-Made Gold Nano-Antennas?

Jan Helbing (Switzerland)

12.40 pm

O IDN 4

Emergence of Raman optical activity spectroscopy as a sensitive tool for lanthanide circularly polarized luminescence

Tao Wu (Czech Republic)

01.00 pm

*lunch*



- 02.00 pm **VII SESSION "APPLICATIONS of VOA - materials"**  
**IS 10**  
**Harnessing electronic and taming structural degrees of freedom in vibrational circular dichroism**  
Wybren Jan Buma (The Netherlands)
- 02.30 pm **IS 11**  
**Intense VCD response of achiral guest Molecules of co-crystalline polymer Films**  
Gaetano Guerra (Italy)
- 03.00 pm **O IDN 18**  
**Sequential induction of chirality in poly(phenylacetylene)s**  
Francisco Javier Ramírez Aguilar (Spain)
- 03.20 pm **POSTER SESSION**
- 04.20 pm *coffee break*
- 04.50 pm **VIII SESSION "APPLICATIONS of VOA – natural products and drugs"**  
**IS 12**  
**Stereochemistry of Natural Cepharanthine Using Chiroptical Spectroscopies**  
Hua-Jie Zhu (China)
- 05.20 pm **IS 13**  
**Vibrational Circular Dichroism in the Pharmaceutical Industry**  
Leo A. Joyce (USA)
- 05.50 pm **IS 14**  
**Model-averaging of ab initio spectra in vibrational Spectroscopy**  
Guglielmo Monaco (Italy)
- 06.20 pm **O IDN 27**  
**Absolute configuration assignment of caffeic acid ester derivatives by VCD: the pitfalls of deuteration**  
João M. Batista Jr. (Brazil)
- 06.40 pm **O IDN 46**  
**Molecular specificity in resonance ROA – B12 vitamin case**  
Agnieszka Kaczor (Poland)

WEDNESDAY September 12<sup>th</sup>

08.30 am Secretariat Desk Opening

*IX SESSION "APPLICATIONS of VOA – proteins, sugars, Lipids and Nucleic Acids; fibrils" part A*

09.00 am IS 15

**Pushing our understanding of the Raman Optical Activity Spectra of Proteins**

Carl Mensch (Belgium)

09.30 am IS 16

**Biomolecules and model membranes by vibrational circular dichroism**

Marie Urbanova (Czech Republic)

10.00 am POSTER SESSION

11.00 am *coffee break*

*CHIROPTICAL SPECTROSCOPIES AND ASTROCHEMISTRY "IN FRONT OF THE MIRROR: THE SEARCH OF CHIRAL MOLECULES IN THE UNIVERSE part A*

11.30 am **Opening Remarks**

Vincenzo Barone

11.35 am IS 17

**title tbd**

Roberto Battiston (Italian Space Agency, Italy)

12.15 pm IS 18

**Mirror molecules and chemistry in the Universe - new challenges and methods**

Melanie Schnell (Germany)

12.45 pm IS 19

**From chiral ACOMS to the origin of life: a quantum chemical and spectroscopic journey**

Cristina Puzzarini (Italy)

01.15 pm *lunch*

**SOCIAL PROGRAMME**

02.30 pm **Guided visit to Santa Giulia Museum**

07.30 pm **Social Dinner**

(Private-Bus Transfer headed to VEDETTA RESTAURANT in Brescia)

THURSDAY September 13<sup>th</sup>

- 08.30 am      **Secretariat Desk Opening**
- 09.00 am      ***X SESSION "General Aspects of Chirality and VOA"***  
**IS 20**  
**Calculating natural optical Activity of helicene Derivatives**  
Monika Srebro-Hooper (Poland)
- 09.30 am      **O IDN 41**  
**Visual exploration of the vibrational chiroptical properties**  
Marco Fusé (Italy)
- 09.50 am      **O IDN 44**  
**DrawMol and DrawSpectrum: new programs to visualize and interpret (optically active) vibrational spectra**  
Vincent Liegeois (Belgium)
- 10.10 am      **O IDN 33**  
**Combinated Vibrational Circular Dichroism and Circularly Polarized Luminescence Studies of Protein Folding**  
Monika Krupová (Czech Republic)
- 10.30 am      *coffee break*
- 11.00 am      ***XI SESSION "APPLICATIONS of VOA – proteins, sugars, Lipids and Nucleic Acids; fibrils" part B***  
**O IDN 12**  
**IR, vcd and ecd spectra, dft simulations, plus MD and T-jump dynamics for three-strand b-sheet peptides. turn and aromatic effects and isotopically edited spectra and dynamics**  
Tim Keiderling (USA)
- 11.20 am      **O IDN 42**  
**Isotopically engendered chirality from enzymatic naphthoyl-ring reduction studied by vibrational circular dichroism**  
Steffen Lüdeke (Germany)
- 11.40 am      **O IDN 7**  
**Supramolecular chirality and enhanced vcd of dna quadruplexes**  
Valery Andrushchenko (Czech Republic)
- 12.00 pm      **O IDN 13**  
**Enhanced VOA as a probe towards intermolecular interactions**  
Evelien Van de Vondel (Belgium)
- 12.20 pm      *lunch*

**CHIROPTICAL SPECTROSCOPIES AND ASTROCHEMISTRY "IN FRONT OF THE MIRROR: THE SEARCH OF CHIRAL MOLECULES IN THE UNIVERSE**

**part B**

01.20 pm

**IS 21**

**title tbd**

Filippo Maria Zerbi (Italian Institute of Astrophysics, Italy)

02.00 pm

**IS 22**

**CH and OH Stretch Vibrations as Probes of Local Environment**

Edwin L. Sibert (USA)

02.30 pm

**IS 23**

**Looking for prebiotic species and chiral molecules in young solar analogs**

Linda Podio (Italy)

03.00 pm

**IS 24**

**Vibrational density matrix renormalization group**

Alberto Baiardi (Switzerland)

03.30 pm

**Closing Remarks**

Sergio Abbate

## CONFIRMED INVITED SPEAKERS

**Alberto Baiardi** - Switzerland  
**Malgorzata Baranska** - Poland  
**Roberto Battiston** - Italy  
**Julien Bloino** - Italy  
**Petr Bour** - Czech Republic  
**Wybren Jan Buma** - The Netherlands  
**Chiara Cappelli** - Italy  
**Gaetano Guerra** - Italy  
**Taka-aki Ishibashi** - Japan  
**Sascha Jähnigen** - Germany  
**Leo A. Joyce** – USA  
**Carl Mensch** - Belgium  
**Guglielmo Monaco** - Italy  
**Linda Podio** - Italy  
**Prasad L. Polavarapu** - USA  
**Dario Polli** - Italy  
**Corina Pollok** - Germany  
**Cristina Puzzarini** - Italy  
**Melanie Schnell** - Germany  
**Edwin L. Sibert** - USA  
**Monika Srebro-Hooper** - Poland  
**Marie Urbanova** - Czech Republic  
**Filippo Maria Zerbi** - Italy  
**Hua-Jie Zhu** - China

## VENUE

**MAIN HALL** of the **SCHOOL OF ECONOMICS** of the **UNIVERSITY OF BRESCIA**  
Via S. Faustino, 74/B – 25122 Brescia (I)

## LOCAL CHAIRMEN

**Prof. Sergio Abbate**  
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**Prof. Vincenzo Barone**  
Pisa (I) - [vincenzo.barone@sns.it](mailto:vincenzo.barone@sns.it)

## ORGANIZING SECRETARIAT

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