

September 23-27 2012  
Palazzo della Carovana  
Scuola Normale Superiore  
Piazza dei Cavalieri, 7  
Pisa

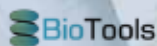


# WORKSHOP CECAM 2012

*VIBRATIONAL OPTICAL ACTIVITY:  
INTERPLAY OF THEORY  
AND EXPERIMENT*



SCUOLA  
NORMALE  
SUPERIORE





**SUNDAY, SEPTEMBER 23<sup>RD</sup> 2012**

18.00-20.00 Registration and Welcome Drink

**MONDAY, SEPTEMBER 24<sup>TH</sup> 2012**

9.00 Opening

**SESSION I**

(9.15-10.35)

Chair: **LAURENCE A. NAFIE**

9.15 **Plenary Lecture:**  
**LAURENCE D. BARRON**  
University of Glasgow, Glasgow, UK  
*Raman Optical Activity. From Discovery to Current Applications*

9.55 **Plenary Lecture:**  
**WERNER HUG**  
University of Fribourg P erolles, Fribourg, Switzerland  
*Mastering the Intricacies of the Measurement and Understanding of ROA Spectra*

10.35 Coffee Break

**SESSION II**

(11.00-13.00)

Philip J. Stephens Memorial Session  
Chair: **RINA K. DUKOR**

11.00 **Plenary Lecture**  
**TIMOTHY KEIDERLING**  
University of Illinois at Chicago, Chicago, USA  
*From CD measurements, Zeeman effects, chiral molecules to biopolymers, solvation and complex systems. Influences of Philip Stephens leading to experimental and theoretical studies of site-specific interactions in peptides and proteins*

11.40 **Plenary Lecture**  
**LAURENCE A. NAFIE**  
Syracuse University, Syracuse, USA  
*Exploring the Origins and Applications of Enhanced Vibrational Optical Activity: From Resonance ROA to VCD of Protein Fibrils*

12.20 **Plenary Lecture**  
**JAMES R. CHEESEMAN**  
Gaussian Inc., Wallingford, USA  
*Theoretical Prediction of Vibrational Raman Optical Activity Spectra*

13.00 Lunch break

### SESSION III

(15.00-16.30)

Chair: **RICCARDO ZANASI**

15.00 **Plenary Lecture**  
**CHRISTOPH JACOB**  
Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany  
*Theoretical Vibrational Spectroscopy with Local Modes*

15.40 **Invited Lecture**  
**PATRICK BULTNICK**  
Ghent University, Ghent, Belgium  
*Absolute configurations using VCD: assignment, comparison to other methods and localizing modes*

16.10 **ESR Talk:**  
**MOJGAN HESHMAT**  
Vrije Universiteit, Amsterdam, The Netherlands  
*On the Equivalence of Conformational and Enantiomeric Changes of Atomic Configuration for Vibrational Circular Dichroism Signs*

16.30 Coffee Break

### SESSION IV

(17.00-18.00)

Chair: **MATTEO TOMMASINI**

17.00 **ESR Talk**  
**JOAO MARCOS BATISTA JR.**  
Sao Paulo State University - UNESP, Araraquara, Brazil  
*VCD to determine the absolute configuration of natural products from Brazilian Cerrado and Atlantic Forest*

- 17.20 **ESR Talk**  
**SHI QIU**  
University of Antwerp, Antwerp, Belgium  
*Identification of diastereoisomers using vibrational circular dichroism versus electric circular dichroism and optical rotatory dispersion: the stereochemistry of tadalafil*
- 17.40 **ESR Talk**  
**VACLAV PROFANT**  
Charles University in Prague, Czech Republic  
*ROA Study of Chondroitin Sulphate and its Building Blocks*
- 18.00 **Poster Session and Cocktail Dinner**

## TUESDAY, SEPTEMBER 25<sup>TH</sup> 2012

### SESSION V

(9.00-10.40)

Chair: **KENNETH RUUD**

- 9.00 **Plenary Lecture**  
**DANIEL CRAWFORD**  
Virginia Tech, Blacksburg, USA  
*Advanced Quantum Mechanical Calculations of Vibrational Effects on Optical Activity*
- 9.40 **Invited Lecture**  
**THOMAS WEYMUTH**  
ETH Zürich, Zürich, Switzerland  
*Theoretical Raman Optical Activity Spectroscopy for Large Molecules*
- 10.10 **Invited Lecture**  
**VINCENT LIEGEOIS**  
FUNDP, Namur, Belgium  
*Pyvib2 as a tool to unravel the vibrational signatures - application to helical systems*
- 10.40 **Coffee Break**

**SESSION VI**

(11.10-12.40)

Chair: **JOANNA SADLEJ**

- 11.10      **Plenary Lecture**  
**VINCENZO BARONE**  
Scuola Normale Superiore, Pisa, Italy  
*A virtual spectrometer for vibrational spectroscopy*
- 11.50      **Invited Lecture**  
**GIOVANNA LONGHI**  
Università di Brescia, Brescia, Italy  
*Harmonic and anharmonic Vibrational Circular Dichroism features of molecules and supramolecular complexes*
- 12.20      **ESR Talk**  
**MAGNUS RINGHOLM**  
CTCC/University of Tromsø, Tromsø, Norway  
*A general open-ended response code*
- 12.40      Lunch break

**SESSION VII**

(14.30-16.20)

Chair: **WOUTER HERREBOUT**

- 14.30      **Plenary Lecture**  
**VOLKER DECKERT**  
University of Jena, Jena, Germany  
*Tip-enhanced Raman Spectroscopy - Current Limits in Spatial Resolution*
- 15.10      **Plenary Lecture**  
**LASSE JENSEN**  
The Pennsylvania State University, USA  
*Plasmon-enhanced chiroptical properties: A combined atomistic electro-dynamics-quantum mechanics model*
- 15.50      **Invited Lecture**  
**ANDRZEJ KUDELSKI**  
University of Warsaw, Warsaw, Poland  
*Local characterisation of surfaces with surface-enhanced Raman spectroscopy*
- 16.20      Coffee Break

**SESSION VIII**

(16.50-18.20)

Chair: **LORENZO DI BARI**

- 16.50    **ESR Talk**  
**STEFFEN LÜDEKE**  
University of Freiburg, Freiburg, Germany  
*Solvent- and Temperature-Dependent Equilibrium of D/L-Configuration in a Tetrahedral Zinc Complex*
- 17.10    **ESR Talk**  
**VALERY ANDRUSHCHENKO**  
Institute of Organic Chemistry and Biochemistry, Prague, Czech Republic  
*Vibrational Circular Dichroism of Nucleic Acids: Combination of Theory and Experiment*
- 17.30    **ESR Talk**  
**ALESSANDRA GIUGLIARELLI**  
University of Perugia, Perugia, Italy  
*VCD as a sensitive probe of solvent effects on protein unfolding and aggregation*
- 20.30    Social Dinner

**WEDNESDAY, SEPTEMBER 26<sup>TH</sup> 2012****SESSION IX**

(9.00-10.50)

Chair: **CHIARA CAPPELLI**

- 9.00-9.40    **Plenary Lecture**  
**MINHAENG CHO**  
Korea University, Seoul, Korea  
*Electric Field Approaches in Chiroptical and Two-Dimensional Optical Spectroscopy*
- 9.40    **Plenary Lecture**  
**IAN R. GOULD**  
Imperial College London, London, UK  
*Potential for the detection of molecular complexes and determination of interaction geometry by 2DIR: Application to protein sciences*

10.20 **Invited Lecture**  
**JAN HELBING**  
Universität Zürich, Zürich, Switzerland  
*Dreams and reality in time-resolved vibrational optical activity measurements*

10.50 Coffee Break

## SESSION X

(11.20-12.30)

Chair: **PETR MALON**

11.20 **Invited Lecture**  
**JOSEF KAPITAN**  
Palacký University in Olomouc, Olomouc, Czech Republic  
*Raman optical activity spectrometer in the deep UV spectral region*

11.50 **ESR Talk**  
**CHRISTIAN MERTEN**  
University of Alberta, Edmonton, Canada  
*Vibrational Circular Dichroism of Matrix Isolated Molecules:  
The Prototype Molecules 3-Butyn-2-ol and Methyl Glycidate*

12.10 **ESR Talk**  
**PAVLINA NOVOTNA**  
Vibrational and electronic circular dichroism for analyzing bilirubin interactions with model membranes

12.30 Lunch break



**SESSION XI**

(14.30-16.10)

Chair: **MAGDALENA PECUL KUDELSKA**

- 14.30 **Plenary Lecture**  
**CHRISTIAN JOHANNESSEN**  
University of Manchester, Manchester, UK  
*Computational Raman optical activity: On the cutting edge*
- 15.10 **Invited Lecture**  
**WYBREN JAN BUMA**  
University of Amsterdam, Amsterdam, The Netherlands  
*Boosting up the difference between left and right*
- 15.40 **Invited Lecture**  
**XYUNJIE XU**  
University of Alberta, Edmonton, Canada  
*Chirality transfer and solvent effects in VCD spectra*
- 16.10 **Coffee Break**

**SESSION XII**

(16.40-18.00)

Chair: **BENOIT CHAMPAGNE**

- 16.40 **Invited Lecture**  
**SERGIO ABBATE**  
Università di Brescia, Brescia, Italy  
*Experimental CPL and Excited State TDDFT Calculations for Camphor and Camphor Derivatives*
- 17.10 **Invited Lecture**  
**ANTONIO RIZZO**  
IPCF-CNR, Pisa  
*Nonlinear in silico spectroscopies turning into novel experiments*
- 17.40 **ESR Talk**  
**SANDRA LUBER**  
Yale University, USA  
*Efficient Calculation of Vibrational Raman Optical Activity Spectra for Bio-and Inorganic Molecules*

**THURSDAY, SEPTEMBER 27<sup>TH</sup> 2012****SESSION XIII**

(9.00-10.50)

Chair: **STEFANO SUPERCHI**

- 9.00 **Plenary Lecture**  
**MICHAEL BARTBERGER**  
Amgen, Inc., Thousand Oaks, California, USA  
*Application of Vibrational Circular Dichroism (VCD) in Industrial Drug Discovery and Development*
- 9.40 **Plenary Lecture**  
**MARIE URBANOVA**  
Institute of Chemical Technology, Prague, Czech Republic  
*Vibrational optical activity induced by interaction of biomolecules*
- 10.20 **Invited Lecture**  
**VLADIMIR BAUMRUK**  
Charles University in Prague, Prague, Czech Republic  
*Raman Optical Activity of Amide and Disulfide Groups in Peptides and Model Systems*
- 10.50 Coffee Break

**SESSION XIV**

(11.20-12.30)

Chair: **FABRIZIO SANTORO**

- 11.20 **Invited Lecture**  
**PAUL NICU**  
Vrije Universiteit, Amsterdam, The Netherlands  
*Interpretation of vibrational circular dichroism spectra*
- 11.50 **Invited Lecture**  
**SONIA CORIANI**  
Università di Trieste, Trieste, Italy  
*Variational response-function formulation of vibrational circular dichroism*
- 12.20 Closing Remarks



Organisers:

**CHIARA CAPPELLI**

Scuola Normale Superiore, Italy

**KENNETH RUUD**

University of Tromsø, Norway

**MAGDALENA PECUL-KUDELSKA**

University of Warsaw, Poland

**RINA DUKOR**

BioTools Inc., USA

<http://www.cecami.org/workshop-636.html>

[http://node.sns.it/workshop\\_vibr](http://node.sns.it/workshop_vibr)

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