

## **EUCMOS 2010 - CONGRESS SITES**

### **Centro Didattico Morgagni**

Viale Morgagni 40, Firenze

### **CTO Conference Hall**

Largo Palagi 1, Firenze

(100 m from Centro didattico Careggi)

### **Palazzo Borghese**

Via Ghibellina 110, Firenze

### **Palazzo Nonfinito**

Via del Proconsolo 12, Firenze

# EUCMOS 2010 - CONGRESS PROGRAMME

## Sunday, August 29 at Palazzo Nonfinito

16.00 - 19.00 Registration

19.00 - 20.00 Welcome Party

## Monday, August 30 at Centro Didattico Morgagni

### MORNING SESSION

**OPENING CERIMONY**      *Room 101 & 109 (109 videoconference)*

8.30 - 9.00      Opening Cerimony

### INVITED LECTURES

9.00 - 9.45      T. W. Haensch  
Spectroscopy with laser frequency combs

9.45 - 10.30      M. Schmitt  
Eigenstate resolved spectroscopy in the gas-phase:  
towards larger systems and higher energies

10.30 -11.00      coffee break

### ORAL PRESENTATIONS

#### *Room 101      Biological and Medical Applications*

11.00 - 11.20      V. Mohaček Grošev, J. Grdadolnik  
Preferred conformations of dipeptides: crystals vs. solutions

11.20 - 11.40      A. Bebu, L. Szabó, N. Leopold, C. Berindean, V. Chiş, L. David  
IR, Raman, SERS and DFT study of amoxicillin

11.40 - 12.00      M. Pučetaitė, V. Hendrixson, A. Želvys, F. Jankevičius, J. Čeponkus, V. Šablinskas  
Highly resolved morphological analysis of renal stones found in mammals using Infrared spectroscopical imaging technique

12.00 - 12.20      A. Torreggiani, Z. Jurasekova, C. Ferreri, C. Chatgililoglu

Effects of radical stress on sulfur-containing proteins: desulfurisation reactions associated with the formation of trans lipids in model membrane

12.20 - 12.40

V. Profant, P. Bouř, V. Baumruk

Formation of PPII helical conformation studied by Raman optical activity

12.40 - 13.00

A. P. Mendham, B. Z. Chowdhry, T. J. Dines

Experimental and theoretical studies of cyclic di-amino acid peptides in the solid state

### **Room 108**

#### ***Materials and Surfaces***

11.00 - 11.20

J. Habinshuti, S. Turrell, C. Kinowski, D. Stievenard, B. Grandidier, T. Xu, O. Cristini

Development of semi-conductor nanoparticle systems for Si-nanowire solar cells

11.20 - 11.40

S. Krawczyk, A. Zdyb, A. Nawrocka

Localized vs charge-transfer excited states of photosensitizers on TiO<sub>2</sub> nanoparticles. Stark effect spectroscopy

11.40 - 12.00

A.M. Yaremko, V.O. Yukhymchuk, V.M. Dzhagan

Spectroscopy study of exciton-phonon interaction in organic and semiconductor quantum dots

12.00 - 12.20

A. Weselucha-Birczyńska, A. Frączek-Szczypta, S. Błażewicz

PAN-based carbon fibers modified with carbon nanotubes

12.20 - 12.40

O. Dammer, B. Vlckova, J. Pflieger, M. Prochazka, M. Slouf

Specific aspects of SERS and SERRS of Ag nanoparticles-polymer nanocomposites

12.40 - 13.00

P. Wilhelm, B. Chernev, H. Plank, M. Sezen, M. Dienstleder, T. Haber, F. Hofer

Raman microprobe imaging of submicron structures and interdisciplinary characterization of beam damage

### **Room 109**

#### ***Spectroscopy and Dynamics: Gas Phase and Matrices***

11.00 - 11.20

E. J. Ocola, A.A. Al-Saadi, J. Laane

Spectroscopic and theoretical investigation of intramolecular  $\pi$ -type hydrogen bonding in 3-Cyclopentenol and related molecules

11.20 - 11.40

L. Rubio-Lago, A. García-Vela, A. Arregui, G. A. Amaral, J. Rodríguez, M. González, L. Bañares

The photodissociation of CH<sub>3</sub>I in the edges of the A-band: Comparison between slice imaging experiments and multisurface wave packet calculations

11.40 - 12.00

R. Flammini, E. Fainelli, L. Avaldi, M. Satta

Dissociation of the ethyne dication: the case of C<sup>+</sup>-H<sup>+</sup>-CH channel

- 12.00 - 12.20 G. Piani, L. Poisson, B. Soep, J.-M. Mestdagh  
Micro-solvation effects in ultrafast relaxation. Application to photochromic molecules
- 12.20 - 12.40 G. B. Poparić, M. M. Ristić, D. S. Belić  
Forward-to-backward differential-cross-section ratio in electron-impact vibrational excitation via the  $^2\Sigma_u^+$  resonance of H<sub>2</sub>
- 12.40 - 13.00 A. Loewenschuss, M. Rozenberg, C. J. Nielsen  
Hydrogen bonding in solid Xenon. A matrix isolation study

13.00 - 14.30 lunch

## AFTERNOON SESSION

### PLENARY LECTURE *Room 101 & 109 (109 videoconference)*

- 14.30 - 15.00 M. Zharnikov  
Characterization of self-assembled monomolecular films by advanced spectroscopic techniques

### ORAL PRESENTATIONS

#### *Room 101 Technical Workshop - ThermoFisher*

- 15.10 - 15.20 T. Locke
- 15.20 - 16.00 B. Beccard  
Applying FT-IR Imaging Microscopy to Biological Tissues Analysis
- 16.00 - 16.30 V. Mussi  
Applying Nanotechnology to Biomedicine: Raman analysis and mapping of carbon nanotubes for drug delivery applications

#### *Room 108 Applied Spectroscopy (cultural heritage, environment, ...)*

- 15.10 - 15.30 B. Zimmermann  
Pollen analysis by transmittance FT-IR spectroscopy
- 15.30 - 15.50 P. Matejka, J. Weissova, Z. Cieslarova, L. Mrnka, M. Clupek, K. Matejkova  
Vibrational spectroscopy as a tool for analysis of tree leaves
- 15.50 - 16.10 S. Osmanoglu, I. Y. Dicle  
Effect of radiation in single crystal of L-glutamine
- 16.10 - 16.30 M. Rudbeck, M. Blomberg, A. Barth  
Environmental effects on phosphorylated amino acids

**Room 109**      ***Spectroscopy and Dynamics: Gas Phase and Matrices***

15.10 - 15.30      M. Coreno, K. Prince

Molecular photoionization spectroscopy with synchrotron radiation

15.30 - 15.50      C. Puzzarini, G. Cazzoli, J. Gauss

Hyperfine structure of rotational spectra: interplay of experiment and theory

15.50 - 16.10      S. Melandri, A. Maris, B.M. Giuliano, L.B. Favero, A. Merloni, W. Caminati

The shape of biomolecules and their weakly bound molecular complexes reviewed by microwave spectroscopy.

16.10 - 16.30      P. R. Joshi, L. Krim

The vibration structure of OH radical and OH-H<sub>2</sub>O complex: A matrix isolation study

16.30 -17.00      coffee break

**Room 101**      ***Technical Workshop - ThermoFisher***

17.00 - 18.00      M. Rocchia, B. Beccard

Hands-on session

**Room 108**      ***Materials and Surfaces***

17.00 - 17.20      A. Gajović, R. Krsmanović, J. Macan, D. S. Su, H. Ivanković

Raman spectroscopy and luminescence of mesoporous ZrTiO<sub>4</sub> ceramics

17.20 - 17.40      A. Rogojanu, C. F. Dascalu, B. C. Zelinschi, D. O. Dorohoi

Electronic absorption spectra of some phtalazinium ylids used to characterize the local ordering processes in liquid and solid solutions

17.40 - 18.00      T. Ishii, H. Kanazawa, S. Kojima

Micro-Brillouin scattering study of orthorhombic HEWL crystals in glycerol

**Room 109**      ***Spectroscopy and Dynamics: Gas Phase and Matrices***

17.00 - 17.20      J. R. Durig, A. Ganguly, S. S. Panikar, I. D. Darkhalil,

T. Iwata

Conformational stability of some organoamines by utilizing Variable temperature infrared spectra of rare gas solutions

17.20 - 17.40      M. Nedić, T. N. Wassermann, R. W. Larsen, M. A. Suhm

Small water/alcohol clusters: a combined Raman- and FTIR-jet study

17.40 - 18.00      S. X. Zhou, J. R. Durig

Conformational stability, structural parameters and vibrational assignment from variable temperature infrared spectra of krypton solution of ethylisocyanate

## Tuesday, August 31 at Centro Didattico Morgagni

### MORNING SESSION

#### INVITED LECTURES *Room 101 & 109 (109 videoconference)*

9.00 - 9.45

D. Anglos

Laser spectroscopies for cultural heritage

9.45 - 10.30

D. D. Bicanic

On a few interesting applications of photothermal science in the characterization of foods

#### PLENARY LECTURE *Room 101 & 109 (109 videoconference)*

10.30 - 11.00

H. Abramczyk

Ultrafast primary events in photostable systems: H-bond, excess electron, biological photoreceptors

11.00 - 11.30 coffee break

### ORAL PRESENTATIONS

#### *Room 101 Materials and Surfaces*

11.30 - 11.50

D. Srankó, M. Sipiczki, É.G. Bajnóczi, M. Darányi, Á. Kukovecz, Z. Kónya, S.E. Canton, K. Norén, P. Sipos, I. Pálinkó

A SEM, EDX and XAS characterization of Ba(II)Fe(III) layered double hydroxides

11.50 - 12.10

M. Handke, M. Gajewicz, A. Kowalewska

Spectroscopy studies of mesotextured cross-linked octahydrodoctasilsesquioxanes materials

12.10 - 12.30

Kh. M. Al-Khamis, Z. Al-Othman, N. M. Al-Andis, R. M. Mahfouz

Kinetic studies for isothermal decomposition of un-irradiated and  $\gamma$ -irradiated gallium acetylacetonate new route for synthesis of gallium oxide nanoparticles

12.30 - 12.50

M. Modreanu

Infrared and Raman spectroscopy investigation of high-k metal oxide thin films: chemical stability, interfacial properties and solid state crystallization

**Room 108** *Applied Spectroscopy (cultural heritage, environment...)*

- 11.30 - 11.50 B. Doherty, C. Miliani, B. G. Brunetti, A. Sgamellotti  
A detachable SERS active polymer film: a minimally invasive approach to the study of painting lakes
- 11.50 - 12.10 M.I. Oshtrakh, M.Yu. Larionov, V.I. Grokhovsky, V.A. Semionkin  
An analysis of Fe and Ni distribution in M1, M2 and M3 sites of iron nickel phosphides extracted from Sikhote-Alin meteorite using Mössbauer spectroscopy with a high velocity resolution
- 12.10 - 12.30 S. Ilieva, D. Cheshmedzhieva, D. Tasheva  
Diastereoselectivity in the Michael addition reaction of CH-acidic Schiff base to  $\alpha,\beta$ -unsaturated ketones
- 12.30 - 12.50 M. Volny, M. Strohmalm, V. Vidova, K. Lemr, J. Pol, M. Hajduch, V. Havlicek  
Mass imaging as a viable 2D alternative for molecular spectroscopists

**Room 109** *Biological and Medical Applications*

- 11.30 - 11.50 S. S. Stavrov  
Carbon monoxide infrared absorption band of carboxyheme proteins as a probe of the protein collective motions.
- 11.50 - 12.10 A. Mezzetti, M. Malferrari, F. Francia, A. Idrissi, G. Venturoli, W. Leibl  
Time-resolved FTIR investigation on light-induced proton-coupled electron transfer reactions in photosynthetic reaction centers
- 12.10 - 12.30 E. Nemtseva, D. Gulnov, M. Gerasimova, V. Kratasyuk  
Fluorescence spectroscopy of the components of the bacterial bioluminescent reaction in viscous media
- 12.30 - 12.50 N. Belogurova, N. Kudryasheva  
Fluorescence features of photoprotein obelin

13.00 - 14.30 lunch

**AFTERNOON SESSION**

**PLENARY LECTURE** Room 101 & 109 (109 videoconference)

14.30 - 15.00 H. H. Mantsch

The renaissance of far infrared spectroscopy, better known as terahertz spectroscopy

## ORAL PRESENTATIONS

### **Room 101**      ***Technical Workshop***

15.10 - 17.10    **Elsevier Science**  
The peer-review system

### **Room 107**      ***Round Table on Computational Spectroscopy***

15.10 - 17.10    **G. Keresztury**, moderator

### **Room 108**      ***Applied Spectroscopy (cultural heritage, environment...)***

15.10 - 15.30    **I. Osticioli, A. Nevin, M. Pagliai, D. Comelli, A. Gallone, G. Valentini, V. Schettino, E.M. Castellucci, R. Cubeddu**

Micro-Raman spectroscopy for the non-destructive molecular characterization of red organic pigments in cross-sections of paintings by Leonardo, Masolino Veronese and Tintoretto

15.30 - 15.50    **D.K. Breiting, G. Brehm, L. Steguweit**

Characterization by vibrational spectrometries of neolithic axe-heads from the Lake Constance region and Northern Switzerland

15.50 - 16.10    **M. Mattarelli, S. Mengon, N. Boschiero, L. Benedetti, F. Deflorian**

Emilio Vedova's paintings: materials and conservation issues

16.10 - 16.30    **T. K. N. Nguyen, K. Bourhis, S. Blanc, E. Péré, C. Vieillescazes**

Solid state complexation of natural organic dyes with Al(III): Electronic and vibrational spectroscopies

16.30 - 16.50    **A. Amat, L. Cartechini, C. Miliani, A. Sgamellotti, S. Fantacci**  
Computational spectroscopy in cultural heritage

### **Room 109**      ***Biological and Medical Applications***

15.10 - 15.30    **H. M. Heise, U. Damm, V. R. Kondepati, R. Kuckuk, J. K. Mader, F. Feichtner, M. Ellmerer**

Infrared spectroscopy in clinical chemistry - from laboratory to continuous patient monitoring

15.30 - 15.50    **G. Steiner, A. Stelling, K. Geiger, E. Koch, R. Salzer, G. Schackert, M. Kirsch**

Vibrational spectroscopy: Towards neurosurgical applications

15.50 - 16.10    **E. Horj, S. Cîntă Pînzaru, C. Soica, C. Dehelean, L. David**

Vibrational spectroscopy characterization of a new pharmaceutical complex of chlorthalidone

16.10 - 16.30 M. Larraona-Puy, A. Ghita, A. Zoladek, W. Perkins, S. Varma, I. H. Leach, A. A. Koloydenko, H. Williams, I. Notingher

Raman micro-spectroscopy as a diagnostics tool for skin cancer detection

16.30-16.50 F.C. Pascut, I. Notingher

Label-free time-course imaging of live cells by confocal Raman micro-spectroscopy

17.10 -17.30 coffee break

## 17. 30 - 19.00 POSTER SESSION 1 - PS1

### Applied Spectroscopy (cultural heritage, environment,...)

- PS1-1 G. Lorenzetti, J. Striova, A. Zoppi, E. M. Castellucci  
Confocal Raman microscopy for in depth analysis in the field of cultural heritage
- PS1-2 S. Dallongeville, M.C. Dhamelincourt, G. Di Lonardo, B. Hernandez, S. Turrell  
Spectroscopic studies of pigment-binder interactions in wall paintings
- PS1-3 O. Cristini, C. Kinowski, S. Turrell  
Micro- Raman spectroscopic study of frescoes from the antiquity period
- PS1-4 N. Stamatovska, P. Makreski, L. Pejov, G. Jovanovski  
Minerals from Macedonia. XXVII. Theoretical and experimental study of the vibrational spectra of Nežilovite
- PS1-5 M. Praisler, D. Domnisoru, S. Gosav  
Multivariate analysis of ancient *Cucuteni* ceramics from Romanian cultural heritage
- PS1-6 W. Mozgawa, M. Król, T. Bajda  
Application of IR spectra in the studies of anion sorption on natural sorbents
- PS1-7 L. Szabó, L.F. Leopold, N. Leopold, I.B. Cozar, V. Chiş

Zn (II) determination in contaminated soil by SERS spectroscopy

- PS1-8**      **S. Salami, E. Péré, G. Lespes**  
Aqueous complexation of humic acid with organostannic compounds by IR spectroscopy and FFF
- PS1-9**      **M. Sitarz, M. Łodziński, A. Pieczka**  
Microprobe analysis and spectroscopic (MIR, Raman and NMR) studies of various members of tourmaline group minerals from Sudety mts, SW Poland
- PS1-10**     **C. F. Dascalu, B. C. Zelinschi, D. O. Dorohoi**  
Main refractive indices of some Carpathian crystals
- PS1-11**     **M. Bartoszek, J. Polak, W. Kapica, W.W. Sułkowski**  
The use of UV/Vis spectroscopy for the estimation of humic acids maturity
- PS1-12**     **G. Trojsi, F. Marazzi, P. Baraldi**  
San Vincenzo al Volturno (Italy) and the identification of blues.
- PS1-13**     **J. Polak, M. Bartoszek, M. Żądło, W.W. Sułkowski**  
The EPR study of humic acid extracted from sediment collected at various seasons
- PS1-14**     **P. Leyton, C. Paipa, A. Zárate, S. Fuentes, R. Sánchez, Y. Leyton**  
Thermal synthesis of Gly-Gln polymer on Rutile. A vibrational study.
- PS1-15**     **M. Žic, M. Ristić and S. Musić**  
Monitoring of hydrothermal precipitation of  $\gamma$ -Fe<sub>2</sub>O<sub>3</sub> from concentrated Fe(NO<sub>3</sub>)<sub>3</sub> solutions partially neutralized with NaOH
- PS1-16**     **A. Adamczyk, W. Mozgawa**  
The influence of different type precursors of Al<sub>2</sub>O<sub>3</sub> and SiO<sub>2</sub> on structure and microstructure of mullite-like gels and coatings
- PS1-17**     **M. Ritz, L. Vaculíková, E. Plevová**  
Identification of clay minerals by infrared spectroscopy and discriminant analysis
- PS1-18**     **M. Ristić, I. Czako-Nagy, S. Musić, A. Vértés**  
Spectroscopic characterization of chrysotile asbestos from different

regions

- PS1-19**     **J. Wąs-Gubała, J. Zięba Palus, B. Trzcińska**  
Microspectrophotometry in visible range as important part of the analysis of coloured forensic traces
- PS1-20**     **J. Zięba Palus, J. Wąs-Gubała**  
An investigation into the use of micro-Raman spectroscopy for the analysis of car paints and single textile fibres
- PS1-21**     **J. Zięba-Palus, A. Michalska, A. Weselucha-Birczyńska**  
Characterisation of paint samples by infrared and Raman spectroscopy for criminalistic purposes
- PS1-22**     **M. Iliut, M. Iosin, S. Astilean**  
Temperature and light-induced effects on milk monitored by fluorescence spectroscopy
- PS1-23**     **L. Bonoldi, C. Flego, L. Montanari**  
The origin of yellowness in Fischer Tropsch waxes studied by molecular spectroscopies.
- PS1-24**     **A. Iordache, E. Horj, M. Culea, O. Cozar**  
Determination of amino acids, fatty acids and selenium in fish plasma by mass spectrometry
- PS1-25**     **Ş. Osmanoglu, Y. Dicle**  
Spectroscopic features of radical induced in gamma irradiated Gabapentin: An EPR Study
- PS1-26**     **P. Mojzeš, J. Palacký, J. Bok**  
SVD-based method for intensity normalization, solvent subtraction and background correction of extensive Raman datasets
- PS1-27**     **B. Zimmermann, G. Baranović**  
Baseline analysis: a simple FT-IR method for obtaining phase transition temperatures
- PS1-28**     **S. Gosav, M. Praisler**  
Optimization of the performances of a hybrid expert system designed for the elucidation of molecular structures

- PS1-29**     **E. Droghetti, C. Focardi, M. Nocentini, G. Smulevich**  
Development of a spectrophotometric method to detect the amount of carbon monoxide in fraudulently treated beef meat
- PS1-30**     **F. Longo, G. Barone, V. Crupi, D. Majolino, P. Mazzoleni, V. Venuti**  
Characterization of archaeological pottery: the case of "Ionic cups"
- PS1-31**     **V. Venuti, G. Barone, V. Crupi, F. Longo, D. Majolino, P. Mazzoleni, D. Tanasi**  
FTIR spectroscopic analysis to study the firing processes of prehistoric ceramics
- PS1-32**     **P. Taddei, G. Freddi, M. Tsukada**  
Vibrational study on the modifications induced by chemical and grafting agents in silk and wool fibres
- PS1-33**     **L. Brambilla, P. Baraldi, L. Toniolo, M.C. Gamberini, S. Goidanich, C. Baraldi**  
Spectroscopic techniques applied to the study of Roman atramenta
- PS1-34**     **M. Pagliai, M. Muniz-Miranda, G. Cardini, V. Schettino**  
Infrared and Raman spectra of minerals from *ab initio* molecular dynamics simulations
- PS1-35**     **G. Perna, M. Lasalvia, P. D'Antonio, G. Quartucci, N. L'Abbate, V. Capozzi**  
Characterization of human cells exposed to deltamethrin by means of Raman microspectroscopy and Atomic Force Microscopy
- PS1-36**     **G. Schettino, P. Cancio Pastor, C. Baffa, E. Giani, M. Inguscio, E. Oliva, A. Tozzi**  
Optical Frequency Comb as the calibration source for the GIANO spectrograph
- PS1-37**     **M. Sitarz, M. Łodziński, M. Kozanecki**  
Spectroscopic and chemical characterization of cavansite and pentagonite from Wagholi, Poonah district, Maharashtra state, India

## Material and Surfaces

- PS1-38**     **M. Kawashima, S. Aramomi, Y. Matsuda, S. Kojima**

Temperature dependence of elastic properties in alkali borate binary glasses

- PS1-39** A. Rogojanu, R. Stanculescu, D. Dorohoi  
Dichroic polymer foils analysed by spectral means
- PS1-40** E. Filip, M. Dulcescu, D. Dorohoi  
Intermolecular interactions in pyridinium ylid ternary protic solutions. theoretical and spectral study
- PS1-41** D. Dorohoi  
Solvent influence on the zwitterionic solutes studied by electron spectroscopy
- PS1-42** J. Pisarska, W.A. Pisarski  
Optical spectroscopy of Dy<sup>3+</sup> ions in heavy metal lead-based glasses and glass-ceramics
- PS1-43** A. Gajović, J. Vukajlović, K. Žagar, M. Plodinec, M. Čeh  
Structural phase transitions of BaTiO<sub>3</sub> nanorods investigated by Raman spectroscopy *in situ* at different temperatures
- PS1-44** C. Bayrak, M.T. Aytekin Aydın  
Vibrational spectroscopic studies on the T<sub>d</sub>-type clathrates: Cd(2,5-dimethylpyrazine)M(CN)<sub>4</sub>·2C<sub>6</sub>H<sub>6</sub> (M= Cd or Hg)
- PS1-45** Ö. Bağlayan, M.T. Aytekin Aydın, M. Şenyel  
Vibrational spectroscopic studies on the Hofmann-type clathrates: M(C<sub>4</sub>H<sub>7</sub>NH<sub>2</sub>)<sub>2</sub>Pd(CN)<sub>4</sub>·2C<sub>6</sub>H<sub>6</sub> (M=Ni, Cd or Co; G=benzene)
- PS1-46** N. Vedeanu, D. A. Magdas, O. Cozar  
IR and 2D correlation spectroscopic investigation of CuO-V<sub>2</sub>O<sub>5</sub>-P<sub>2</sub>O<sub>5</sub>-CaF<sub>2</sub> glass system
- PS1-47** R. Dēdic, V. Vyklický, A. Svoboda, J. Hála  
Singlet Oxygen photosensitization in polymer films
- PS1-48** R. Dēdic, V. Vyklický, J. Hála  
Dependence of Singlet Oxygen kinetics on photosensitizer concentration in lipid films
- PS1-49** M. Alloisio , A. Demartini , S. Leporatti , A. Rindi , C. Cuniberti ,

**G. Dellepiane, G. Margheri, E. Giorgetti, M. Muniz-Miranda**  
Spectroscopic investigation on noble metal-organic nanohybrids with controlled shapes and properties

- PS1-50** **T. V. Tran, S. Turrell, C Kinowski, O. Cristini, B. Capoen, M. Bouazaoui, P. Roussel, S. Berneschi, G. Righini, M. Ferrari, S.N. B. Bhaktha**  
Kinetics of crystallization of SnO<sub>2</sub> nanoparticles in sol-gel -based glass ceramics: comparison of thin films and bulk systems
- PS1-51** **C. Zimmerer, G. Steiner, V. Sablinskas, G. Heinrich**  
Nanoparticle enhanced FTIR spectroscopy of polymer interfaces
- PS1-52** **O. Ryazanova, I. Voloshin, V. Zozulya**  
Spectroscopic study of tetracationic porphyrin H-aggregation on polyanionic matrix
- PS1-53** **S. Rada, V. Dan, M. Rada, M. Culea, T. Rusu, M. Bosca, L. Pop, E. Culea**  
FTIR, UV-VIS spectroscopy and DFT calculations on the structure of the gadolinium-lead-germanate glasses
- PS1-54** **R. Chelcea, S. Rada, E. Culea**  
FTIR, UV-VIS and EPR spectroscopy investigations of the copper-lead-germanate glasses
- PS1-55** **S. Rada, R. Chelcea, A. Dehelean, P. Pascuta, T. Ristoiu, I. Coroiu, M. Barlea, E. Culea**  
FTIR, UV-VIS and EPR investigations of the gadolinium-lead-tellurate unconventional glasses
- PS1-56** **A. Dehelean, S. Rada, E. Culea**  
Redox processes in iron-lead-tellurate glasses
- PS1-57** **M. Rada, V. Maties, S. Rada, I. V. Simiti, E. Culea**  
Novel photochromic properties of the tungsten-lead-borate glasses
- PS1-58** **M. Gotić and S. Musić**  
Hydrothermal synthesis of Iron Oxide nanorings by Mn-doping
- PS1-59** **M. Vyskovska, V. Prokopec, M. Clupek, A. Kokaislova, J. Cejkova, P. Matejka**

Development of copper nanostructured materials for surface-enhanced Raman scattering spectroscopy

- PS1-60**     **D. Bauman, N. Bielejewska**  
Molecular aggregation of naphthalimide dyes in Langmuir-Blodgett films
- PS1-61**     **R. Stanescu, N. Vedeanu, S. Filip, O. Cozar**  
EPR and IR structural investigation of  $V_2O_5 - P_2O_5 - BaO$  glass system with opto-electronic potential
- PS1-62**     **P. Angelova, N. Kuchukova, G. Dobrikov, I. Petkova, E. Giorgetti, I. Timtcheva, K. Kostova, E. Vauthey**  
Preparation and photophysical study of fluorophore modified Gold nanoparticles
- PS1-63**     **M. Plodinec, D. Iveković, D. Su, A. Gajović.**  
*In situ* high temperature Raman spectroscopy of modified titanate nanotubes
- PS1-64**     **M. Handke, M. Sitarz, E. Długoń**  
FT-IR and MAS-NMR spectra of  $SiC_xO_y$  glass materials
- PS1-65**     **L. Mikac, M. Ivanda, G. Štefanić, S. Musić, K. Furić**  
Spherical vibrational modes of amorphous and crystalline  $ZrO_2 - CuO$  nanoparticles
- PS1-66**     **M. Ivanda, M. Balarin, O. Gamulin, V. Đerek, D. Ristić, S. Musić, M. Ristić, and K. Furić**  
Porous silicon prepared by electrochemical etching of silicon epitaxial layer
- PS1-67**     **D. A. Magdas, N. Vedeanu, O. Cozar**  
Spectroscopic studies of  $Mo-Cu-Pb-P_2O_5$  glass system
- PS1-68**     **D. Mikociak, C. Paluszkiwicz, S. Błażewicz**  
FTIR spectroscopy analysis of oxidation process of coal tar pitches
- PS1-69**     **D. Rusu, A. R. Tomsa, M. H. Dickman, U. Kortz, O. Baban, M. Rusu**  
Synthesis and characterization of the novel heteropolyoxotungstates based on  $[BiW_9O_{33}]^{9-}$  units

- PS1-70**     **Z. Csendes, N. Földi, N. Varga, J.T. Kiss, I. Labádi, I. Pálinkó**  
Covalently grafted, silica gel supported mixed amino acid iron complexes – syntheses, structural characterization and catalytic testing
- PS1-71**     **M. Balarin, O. Gamulin, M. Ivanda, M. Kosović, D. Ristić, M. Ristić, S. Musić, K. Furić**  
Optical properties of porous silicon on an insulator layer
- PS1-72**     **I. Bryndal, E. Kucharska, K. Hermanowicz, M. Mączka, M. Wandas, J. Hanuza**  
The crystal and molecular structure of new hybrid material: 2-amino-4-methyl-3-nitropyridinum hydrogen oxalate
- PS1-73**     **D. Ristić, V. Holy, M. Ivanda, M. Marciuš, M. Buljan, O. Gamulin, K. Furić, M. Ristić, S. Musić, M. Mazzola, A. Chiasera, M. Ferrari, G.C. Righini**  
Surface characterisation of thin silicon rich oxide thin films
- PS1-74**     **A. Šarić, S. Musić, M. Ivanda**  
Varying the microstructural properties of ZnO particles using different synthesis routes
- PS1-75**     **M. Maczka, M. Ptak, W. Paraguassu, P.T.C. Freire, A.G. Souza Filho, J. Mendes Filho, J. Hanuza**  
Lattice dynamics and high-pressure Raman scattering studies of cation-deficient Aurivillius compounds
- PS1-76**     **W. Paraguassu, M. Maczka, K. Pereira da Silva, A. G. Souza Filho, P.T.C. Freire, J. Mendes Filho, and J. Hanuza**  
Vibrational properties of hexagonal bronze systems: High pressure and polarized Raman spectra
- PS1-77**     **W. Makulski**  
Reconsideration of the  $^{13}\text{C}$  absolute nuclear magnetic shielding scale from NMR measurements of CO/He and CH<sub>4</sub>/He gas phase mixtures
- PS1-78**     **M. Ziabka, C. Paluszkiwicz, J. Chlopek**  
FTIR study of PGLA modified with nanoadditives
- PS1-79**     **W. Pohle, D.R. Gauger, E. Mrazkova, P. Hobza**

Headgroup hydrocarbon groups are involved in water binding as revealed by isotope IR spectroscopy

- PS1-80**     **A. Nyczyk, C. Paluszkiwicz, M. Hasik**  
Polysiloxane networks formation studied by FTIR spectroscopy
- PS1-81**     **C. Paluszkiwicz, E Sottysiak, M. Blazewicz**  
Characterization of ceramic/poly- $\epsilon$ -caprolactone nanocomposite materials by FTIR spectroscopy
- PS1-82**     **M. Piccardo, M. Ottonelli, D. Duce, S. Thea, G. Dellepiane**  
Tuning the photophysical properties of pyrene-based systems: a theoretical study
- PS1-83**     **A. Rindi, G. Margheri, M. Muniz-Miranda, G. Dellepiane, M. Alloisio**  
Metal-organic platforms for photonic applications based on poly-10,12 dicosadiynedioic acid (PDCDA)
- Vibrational and Electronic Spectroscopy**
- PS1-84**     **S. A. Brandán, E. Eroğlu, A. E. Ledesma, O. Oltulu, O. B. Yalçinkaya**  
DFT molecular force field of acetazolamide compound
- PS1-85**     **Z. Dega-Szafran, A. Katrusiak, M. Szafran, P. Barczyński**  
Spectroscopic and structural studies of 2-(quinuclidinium)-butyric acid bromide hydrate
- PS1-86**     **N. Eremina, A. Barth**  
Infrared spectroscopic studies of  $\text{Ca}^{2+}$  ATPase phosphoenzyme
- PS1-87**     **M. Samsonowicz, E. Regulska, R. Świsłocka, W. Lewandowski**  
Experimental and theoretical study of molecular structure of magnesium, calcium, strontium and barium 4-nitrobenzoates
- PS1-88**     **A. Gatiał, H. Juhásová, M. Gróf, J. Kožíšek, V. Milata, N. Prónayová, P. Matějka**  
Isomerizational and conformational study of methyl-2-cyano-3-methoxyacrylate (MCMA) and methyl-2-cyano-3-aminoacrylate (MCAA) and its N-methyl derivatives
- PS1-89**     **V. Sablinskas, I. Doroshenko, V. Pogorelov, V. Balevicius**

Propanol in argon matrix: 2D FTIR correlation spectroscopy

- PS1-90**     **A. Şengül and E. Eroğlu**  
Vibrational and structural study of 6,6'-diacetyl-2,2'-bipyridine dioxime using FT-IR Raman and quantum chemical calculations
- PS1-91**     **N. Vedeanu, A. Pîrnău, B. I. Cozar, O. Oniga, C. Moldovan, C. M. Lucaciu**  
NMR, IR and Raman investigation of 3-[2-(4-Methyl-2-phenyl-thiazol-5-yl)-2-oxo-ethyl]-thiazolidine-2,4-dione compound with antimicrobial potential
- PS1-92**     **M.M. Szostak, K. Piela, H. Chojnacki, E. Bidzińska, K. Dyrek**  
Paramagnetic species generated by near IR as possible intermediates in molecular mechanism of optical nonlinearity in 1,3-dinitrobenzene crystal. NIR, EPR, CD and quantum chemical studies
- PS1-93**     **F. Kollipost, S. Hesse, J. J. Lee, M. A. Suhm**  
Dimers of cyclic carbonates: Chirality recognition in battery solvents
- PS1-94**     **M. Citroni, R. Bini, M. Pagliai, G. Cardini, V. Schettino**  
The reactivity of nitromethane under high static pressure
- PS1-95**     **A. Maris, S. Melandri, W. Caminati, L. B. Favero**  
Rotational spectrum of glycolamide-water and glycolamide-ammonia molecular complexes.
- PS1-96**     **A. Mayer, M. Sipiczki, Gy. Szöllösi, J.T. Kiss, I. Pálinkó**  
Synthesis, structural characterization and some applications of immobilized organocatalysts
- PS1-97**     **I.B. Cozar, L. Szabó, N. Leopold, D. Mare, V. Chiş, L. David**  
Vibrational spectroscopic and DFT study of paroxetine
- PS1-98**     **M. Kurt and H. Yurtseven**  
Analysis of the frequency shift and the linewidth as a function of temperature in solid nitrogen
- PS1-99**     **C. Ivascu, L. Daraban, O. Cozar, I. Ardelean**  
FT-IR and Raman studies on the P<sub>2</sub>O<sub>5</sub>-BaO-Li<sub>2</sub>O glass system
- PS1-100**    **S. Demirci, S. Kınalı, Z. Çalışır, M. Kurt, A. Ataç**

DFT, FT-Raman, FT-IR and NMR studies of 4-(substituted phenylazo)-3,5-diacetamido-1H-pyrazoles

- PS1-101** G. Ogruc-Ildiz  
Theoretical and experimental vibrational analysis of Hydantion
- PS1-102** M. Nedić, M. Albrecht, B. Dittrich, M. A. Suhm  
Methyl Mandelate - From dimers to crystals
- PS1-103** N. O. B. Lüttchwager, T. N. Wassermann, S. Coussan, M. A. Suhm  
Environmental and vibrational influence on the proton transfer in malonaldehyde
- PS1-104** A. Bebu, A. Kozma, E. Forizs, M. Toderas, L. David  
Spectral and ESR study of Cu(II), Co(II) and Ni(II) theophyllinato complexes containing propanolamine ligands
- PS1-105** S. Akyuz T. Akyuz  
Adsorption of 2- and 3-Chloropyridine on Sepiolite and Loughlinite: An Infrared spectroscopic study
- PS1-106** E. L. Terpugov, O. V. Degtyareva  
Mid-infrared stimulated emission spectroscopy and its Applications
- PS1-107** I. Kowalczyk, M. Szafran  
Aminopyridine betaines and their hydrohalides studied by FTIR and NMR spectroscopy and DFT calculations
- PS1-108** M. E. Defonsi Lestard, L. A. Ramos, M.E. Tuttolomondo, S. E. Ulic, A. Ben Altabef  
Synthesis, spectroscopic and structural properties of trichloromethyl trifluoromethanesulphonate,  $CF_3SO_2OCCl_3$
- PS1-109** A. Pîrnău, M. Bogdan, M. Palage, L. Szabo, N. Leopold, R. A. Varga, O. Cozar, V. Chiş  
Experimental and theoretical investigation of 2-phenyl-thiazole-4-yl-methyl-quinolinium iodine
- PS1-110** M. Ptak, M. Maczka, J. Hanuza, A. A. Kaminskii, P. Becker, L. Bohaty  
Raman and IR studies of melilite-type crystals  $Ca_2MgSi_2O_7$ ,  $Ca_2ZnSi_2O_7$

and  $\text{Sr}_2\text{MgSi}_2\text{O}_7$

- PS1-111** J. Lorenc  
Effect of methyl group and N-H...N hydrogen bond on IR and Raman spectra of 2-(N-ethylamino)- 3(or 5)-methyl-4-nitropyridine
- PS1-112** L. Illés, K. Felföldi, J.T. Kiss, I. Pálinkó  
C-H...S hydrogen bonds as the organizing force in 2,3-thienyl- and phenyl- or 2,3-dithienyl-substituted propenoic acid aggregates studied by the combination of FT-IR spectroscopy and computations
- PS1-113** A. A. Yakubov  
Hydrogen bonds and mesomorphism of cholesteryl formiate
- PS1-114** V. M. Petruševski, D. Sazdov, B. Šoptrajanov  
The O-D/HDO stretchings in the  $\text{Li}_2(\text{S,Se})\text{O}_4 \cdot (\text{H,D})_2\text{O}$  system: employing the double isolation method
- PS1-115** T. Jednačak, P. Novak, A. Kišić, T. Hrenar, S. Miljanić G. Verbanec  
Reaction monitoring of entacapone synthesis by in-line Raman spectroscopy and principal component analysis
- PS1-116** N.P.C. Westwood, J. Wang  
Cyanogen isocyanate, NCNCO; the infrared conundrum
- PS1-117** N.F.L. Machado, L.A.E. Batista de Carvalho M.P.M. Marques  
Antioxidant chromones - A conformational study
- PS1-118** O. Gamulin, M. Ivanda, V. Mitsa, M. Balarin, and M. Kosović  
Monitoring of structural phase transition of  $(\text{Ge}_2\text{S}_3)_x (\text{As}_2\text{S}_3)_{1-x}$  chalcogenide glass with Raman spectroscopy
- PS1-119** A. Lucotti, M. Tommasini, W.A. Chalifoux, D. Fazzi, G. Zerbi, R.R. Tykwinski  
Bent polyynes: Ring strain studied by Raman and Infrared spectroscopies
- PS1-120** R.M. Lees, Li-Hong Xu, B.E. Billingham  
Weeding the Cosmos - FTIR synchrotron spectroscopy of Methanol isotopologues at the Canadian light source

- PS1-121** A. Weselucha-Birczyńska, T. Toboła  
Raman microspectroscopy of inclusions in bituminous salts
- PS1-122** G. Štefanić, I. I. Štefanić, S. Musić and M. Ivanda  
Structural and microstructural changes in the zirconium-indium mixed oxide system during thermal treatment
- PS1-123** P. Barczyński, M. Szafran  
Structure of 3,4-dicarboxy-1-methylpyridinium betaine studied by X-ray diffraction, DFT calculations, NMR and FTIR spectra
- PS1-124** A. Esme, S. Sagdinc  
The studies of molecular structures and vibrational spectra of Sudan Orange G and Sudan Red G
- PS1-125** K. Chruszcz-Lipska, A. Kaczor  
Structural behavior of selected ionones upon thermal stress conditions
- PS1-126** B. M. Giuliano, I. Reva, R. Fausto, S. Melandri  
Infrared spectroscopy and photochemistry of 2-phenylethylamine and its derivatives isolated in noble gas matrices.
- PS1-127** C. M. Nunes, I. Reva, R. Fausto, T. M.V.D. Pinho e Melo  
Flash vacuum pyrolysis of Isoxazole. A low temperature matrix isolation Infrared spectroscopy study.
- PS1-128** A. Sharma, N. Kuş, I. Reva, L. Lapinski, R. Fausto  
Infrared spectra of matrix-isolated 4-methoxybenzaldehyde (*p*-anisaldehyde) conformers
- PS1-129** I. Doroshenko, V. Pogorelov, P. Uvdal, V. Balevicius, V. Sablinskas  
Temperature controlled kinetics of growing and relaxation of alcohol clusters in Argon matrix
- PS1-130** I. Reva, L. Lapinski, R. Fausto  
Spectral indicators of structural flexibility of matrix isolated methyl isocyanate
- PS1-131** M. Rozenberg, A. Loewenschuss  
The matrix isolation Infrared spectrum of the Sulfuric Acid-monohydrate complex: New assignments and resolution of "missing H-bonded  $\nu(\text{OH})$  band" issue.

- PS1-132**    **N. Kuş, I. Reva, R. Fausto**  
Infrared spectrum and photochemistry of matrix-Isolated 3-Furaldehyde
- PS1-133**    **J. Dobrowolski, M. H. Jamróz, R. K., J. E. Rode, M. K. Cyrański, J. Sadlej**  
IR low-temperature matrix, X-ray and ab initio study on L-Isoserine conformations
- PS1-134**    **M. Ceppatelli, S. Fanetti, M. Citroni, R. Bini**  
Photoinduced reactivity of liquid ethanol at high pressure

## Wednesday, September 1 at Centro Didattico Morgagni

### MORNING SESSION

#### INVITED LECTURES *Room 101 & 109 (109 videoconference)*

- 9.00 - 9.45      **J. M. Thomas**  
The confluence of spectroscopy, microscopy and tomography
- 9.45 - 10.30    **M. Zanni**  
Watching proteins aggregates and electron transfer with 2D-IR spectroscopy
- 10.30 - 10.40   **GISR 2010: welcome to participants**

#### PLENARY LECTURE *Room 101 & 109 (109 videoconference)*

- 10.40 - 11.10   **C. Castiglioni**  
Raman evidences of unusual electronic and molecular structures

11.10 -11.40    **coffee break**

### ORAL PRESENTATIONS

#### *Room 101      Biological and Medical Applications*

- 11.40 - 12.00    **O.F. Nielsen, T.M. Greve, A. Engdahl**  
FTIR-synchrotron and NIR-FT-Raman studies of water in animal and human skin
- 12.00 - 12.20    **T. Pazderka, V. Kopecký Jr., K. Hofbauerová, V. Baumruk**  
Two-dimensional Raman and Raman optical activity correlation and factor analysis of lysozyme fibrillation
- 12.20 - 12.40    **M. Talu, E. Uzluk**  
Synthesis and characterization of antibacterial Poly(N-vinylimidazole-co-maleic anhydride)/Sodium Bentonite composites
- 12.40 - 13.00    **K. Hauser, C. Krejtschi, O. Ridderbusch, R. Huang, L. Wu, T. A. Keiderling**  
Folding dynamics of hairpin peptides studied by temperature-jump infrared-spectroscopy and isotopic editing

#### *Room 108      Materials and Surfaces*

- 11.40 - 12.00 **K. Csankó, M. Darányi, G. Kozma, Á. Kukovecz, Z. Kónya, I. Pálinkó**  
Self-assembling of Z- $\alpha$ -pyridylcinnamic acid dimers over polycrystalline Ag and Au surfaces followed by FT-IR and atomic force microscopies
- 12.00 - 12.20 **R. Stiufiuc, B. Grandidier, G. Stiufiuc, C. M. Lucaciu**  
STM/STS characterization of PTCDI/melamine self assembly on Si(111)  $\sqrt{3} \times \sqrt{3}$  Ag surface
- 12.20 - 12.40 **W. Pohle, D.R. Gauger, V. Andrushchenko, P. Bouř, F. Billes**  
A spectroscopic method to estimate the binding potency of amphiphile assemblies
- 12.40 - 13.00 **Do Thi Minh, K. Volka**  
Vibrational spectroscopy in the study of self-assembled monolayers of thiols on gold. An example of 4-mercaptobenzoic acid

**Room 109 GISR**

- 11.40 - 12.00 **E. Collini, G.D.Scholes**  
Coherent dynamics in energy migration at room temperature: Evidence for subtle quantum-mechanical strategies for energy transfer optimization
- 12.00 - 12.20 **E. Garbin, E. Lubian, S. Kovalenko, N. Ernsting, T. Carofiglio, C. Ferrante**  
Energy transfer processes in homo and hetero dimers of porphyrins
- 12.20 - 12.40 **H. Torii, M. G. Giorgini, M. Musso**  
One- and two-mode behavior of the  $\nu(\text{C}=\text{O})$  band in N,N-dimethylformamide isotopic mixtures: DMF/DMF- $d_6$  and DMF/DMF- $^{13}\text{C}$ O
- 12.40 - 13.00 **A. Lapini, P. Tourón Touceda, S. Mosquera Vazquez, M. Lima, A. Dei, P. Foggi, R. Righini**  
Transient Infrared spectroscopy: A new approach to investigate valence tautomeric interconversion

13.00 - 14.30 lunch

**EUCMOS CONFERENCE EXCURSION****AFTERNOON SESSION (GISR)**

**ORAL PRESENTATIONS****Room 109**      ***GISR: a view of selected posters***

- 14.30 - 14.50    **C. Lofrumento**, Ph. Sciau, Y. Leon, E. M. Castellucci  
A semi-quantitative LIBS analysis on *Terra Sigillata* wares
- 14.50 - 15.10    **G. Das, M.L. Coluccio, A. Nicastrì, F. Gentile, F. De Angelis, E. Di Fabrizio, G. Cuda**  
Raman spectroscopy for the evaluation of structural changes of peptides
- 15.10 - 15.30    **M. Ceppatelli**, R. Bini, V. Schettino  
High pressure photoinduced reactivity in clathrate hydrates
- 15.30 - 15.50    **S. Abbruzzetti, A. Bonamore, A. Boffi, A. Feis, P. Foggi, C. Gellini, A. Marcelli, P.R. Salvi, C. Viappiani**  
Time-resolved spectroscopy of native and mutated *Thermobifida fusca* hemoglobins
- 15.50 - 16.10    **B. M. Giuliano, V. Feyer, K.C. Prince, M. Coreno, L. Evangelisti, S. Melandri, W. Caminati**  
Tautomerism in pyrimidine derivatives investigated with core level spectroscopy techniques

16.10 -16.40      **coffee break**

- 16.40 - 17.00    **M. Biczysko**  
Computational spectroscopy as a tool to interpret experimental results: From small molecules in the gas phase to large systems in condensed phases.
- 17.00 - 17.20    **V. Amendola, G. Marcolongo, G. Fracasso, M. Colombatti and M. Meneghetti**  
SERS active gold nanostructures for selective and ultrabright biolabelling: Synthesis and quantitative study
- 17.20 - 17.40    **P. Taddei, E. Modena, A. Tinti, F. Siboni, C. Prati, M.G. Gandolfi**  
Vibrational investigation on the in vitro bioactivity of commercial and experimental calcium-silicate cements for root-end endodontic therapy

17.40 - 19.00    ***GISR Round Table***

**Thursday, September 2**  
**Morning at CTO Conference Hall**  
**Afternoon at Centro Didattico Morgagni**

**MORNING SESSION at CTO Conference Hall**

**INVITED LECTURES**

- 9.00 - 9.45      **P. Hildebrandt**  
Raman and IR spectroscopic approaches for studying protein structure and dynamics
- 9.45 - 10.30    **J. V. Garcia Ramos**  
New approaches in metal enhanced spectroscopy (SERS and SEF) in solution: Detection of insoluble compounds and pharmaceutical drugs

**PLENARY LECTURE**

- 10.30 - 11.00    **M.S. Pshenichnikov**  
2D IR spectroscopy of water dynamics near hydrophobes

11.00 - 11.30    **coffee break**

**11.30 - 13.30    POSTER SESSION 2 - PS2**

***Biological and Medical Applications***

- PS2-1      **E. Droghetti, M. Zamocky, P.G. Furtmüller, C. Obinger, G. Smulevich**  
Resonance Raman spectroscopy of catalase-peroxidase from the phytopathogenic rice blast fungus *Magnaporthe grisea*
- PS2-2      **M.I. Oshtrakh, I.V. Alenkina, S.M. Dubiel, V.A. Semionkin**  
Structural variations of the iron cores in human liver ferritin and its pharmaceutically important models: a comparative study using Mössbauer spectroscopy with a high velocity resolution
- PS2-3      **M.I. Oshtrakh, A. Kumar, S. Kundu, A.L. Berkovsky, V.A. Semionkin**  
Study of human, rabbit and pig oxyhemoglobins using high velocity

resolution Mössbauer spectroscopy in relation to its structural and functional variations

- PS2-4 **V. Šablinskas, V. Urbonienė, E. Kaveckaitė, F. Jankevičius, G. Steiner, L. Kintys**  
Infrared spectral microscopy of cancerous kidney tissues
- PS2-5 **H. Abramczyk, B. Brożek-Płuska, J. Surmacki, J. Jabłońska, R. Kordek**  
The label-free Raman imaging of human breast cancer
- PS2-6 **T. Yasui, T. Araki**  
Visualization of collagen molecule orientation in wrinkled skin using a polarization-resolved second-harmonic-generation microscope
- PS2-7 **M. Sefa Ozel, A. E. Ozel, S. Akyuz, T. Akyuz**  
Combined micro-Raman and EDXRF study of characterization of mineralized tissue of human bone of osteoporosis patients
- PS2-8 **C. Paluszkiwicz, E. Stodolak, J.W.M.Kwiatek, P. Jeleń**  
Bioactivity of montmorillonite - chitosane nanocomposite materials for regenerative medicine
- PS2-9 **L. Bednárová, P. Maloň, H. Dlouhá, M. Kubáňová, P. Mojzeš, E. Kočíšová, K. Hofbauerová, V. Kopecký Jr.**  
Antibacterial peptides in interaction with model membranes studied by various spectroscopic methods
- PS2-10 **A. Falamas, S. Cinta Pinzaru, C. Dehelean, A. Bebu**  
Spectroscopic investigations of newly formed guest-host type complexes as potential anti skin cancer candidates
- PS2-11 **J. Równicka-Zubik, A. Sułkowska, E. Kurek, M. Maciążek-Jurczyk, B. Bojko, W. W. Sułkowski**  
The comparison of the binding properties of native and destabilized serum albumins
- PS2-12 **M. Maciążek-Jurczyk, A. Sułkowska, B. Bojko, J. Równicka-Zubik, W. W. Sułkowski**  
Polypharmacotherapy in rheumatology. <sup>1</sup>HNMR analysis of binding of phenylbutazone and methotrexate to serum albumin

- PS2-13**     **M. Di Foggia, E. Benassi, S. Bonora, S. Ottani**  
Vibrational (Raman and SERS) and electronic UV study on triazine herbicides
- PS2-14**     **I. B. Cozar, L. Szabó, O. Cozar, N. Leopold, V. Chiş, L. David**  
IR, SERS and DFT Study of Pindolol and Verapamil Drugs
- PS2-15**     **B. Brycki, I. Kowalczyk, A. Szulc**  
Spectroscopic analysis of gemini alkylammonium salts with the antimicrobial activity
- PS2-16**     **A. Hense, A-K. Mossberg, C. Svanborg, A. Barth**  
Infrared spectroscopic study of HAMLET, a tumor-killing variant of  $\alpha$ -lactalbumin
- PS2-17**     **P. Maloň, L. Bednárová, M. Kubáňová, M. Flegel, J. Hlaváček, V. Baumruk**  
Vibrational and electronic optical activity of amide and disulfide groups in neurohypophyseal hormones and their models
- PS2-18**     **N. Mironova-Ulmane, M. Polakovs, A. Pavlenko, N. Kurjane, E. Reinholds, M. Grube**  
Spectroscopic study of blood after irradiation
- PS2-19**     **P. Praus, E. Kočíšová, P. Mojzeš, J. Štěpánek, F. Sureau, P.-Y. Turpin**  
Cellular uptake of modified oligonucleotides enhanced by zinc porphyrins studied by time-resolved micro-spectrofluorimetry and fluorescence imaging techniques
- PS2-20**     **S. Boca, D. Rugina, A. Pinteá, L.-B. Tudoran, S. Astilean**  
Synthesis and characterization of flower-shaped gold nanoparticles for applications as SERS-active tags in cellular spectral imaging
- PS2-21**     **S. Akyuz, A. E. Ozel, K. Balci, T. Akyuz, A. Coker, E. D. Arisan, N. Palavan-Unsal, A. Ozalpan**  
Micro Raman spectroscopic investigation of the interaction of cultured HCT116 colon cancer cells with  $\alpha$ -difluoromethylornithine (DFMO), an irreversible inhibitor of ornithine decarboxylase
- PS2-22**     **L. Andronie, S. C. Pînzaru, O. Cozar**  
Surface-enhanced Raman scattering of DL-tryptophan

- PS2-23 **A. Torreggiani, M. Di Foggia, A. Tinti**  
Investigations on metallothioneins: An help from Raman spectroscopy
- PS2-24 **J. Kaminsky, J. Kubelka, P. Bour**  
Theoretical models for better understanding of IR and CD spectra of proteins
- PS2-25 **M. Śmiechowski, E. Gojto, J. Stangret**  
Hydration of simple carboxylic acids from infrared spectroscopy of HDO
- PS2-26 **M. Grube, M. Gavare, R. Rutkis, U. Kalnenieks, N. Mironova-Ulmane**  
Use of FT-IR spectroscopy data for systems analysis of *Zymomonas mobilis* metabolism
- PS2-27 **P. Ottová, B. Řezáčová, J. Vachoušek, J. Štěpánek**  
Structural stability and complexation with aptamers of RNA hairpins in HIV-1 genome
- PS2-28 **F. Torrens, G. Castellano**  
Binding of proteins to vesicles: Asymmetry and cooperativity
- PS2-29 **G. Petruševski, S. Ugarkovic, P. Makreski**  
Solid-state transformation of the pseudopolymorphic forms of codeine phosphate hemihydrate and codeine phosphate sesquihydrate monitored by FTIR spectroscopy and TGA/DSC
- PS2-30 **R. Świśtocka, M. Kalinowska, W. Ferenc, J. Sarzyński, W. Lewandowski**  
Spectroscopic and magnetic properties of Cu(II) complexes with selected biologically important ligands
- PS2-31 **M. Kalinowska, J. Piekut, W. Lewandowski**  
Relationship between chemical structure and biological activity of alkali metal *o*-, *m*- and *p*-anisates. FT-IR and microbiological studies
- PS2-32 **M. Potara, S. Astilean**  
Solution-phase, dual LSPR-SERS plasmonic sensors of high sensitivity and stability based on chitosan-coated anisotropic silver nanoparticles

- PS2-33**     **M. Kubáňová, L. Bednářová, P. Maloň, V. Baumruk**  
Raman optical activity of amide and disulfide group in peptides and proteins
- PS2-34**     **A. Tinti, G. Navarra, M. Leone, V. Militello, A. Torreggiani**  
Influence of metal ions on thermal aggregation processes of globular proteins
- PS2-35**     **A. Wesełucha-Birczyńska, B. Borzęcka-Prokop**  
Compound formation assistance by Raman spectroscopy and PXRD method
- PS2-36**     **P.T.C. Freire, R.O. Holanda, C. Luz-Lima, J. Mendes Filho, F.E.A. Melo**  
Raman spectroscopy of L-glutamine under high pressure conditions
- PS2-37**     **A. Pallagi, P. Sebők, P. Sipos, I. Pálinkó**  
Structure-reactivity relationship of Ca<sup>2+</sup>-carbohydrate solution complexes studied by H, <sup>13</sup>C and <sup>43</sup>Ca NMR spectroscopy
- PS2-38**     **K. Balci, Y. Akkaya, S. Akyuz, N. Palavan-Unsal**  
An IR and Raman spectroscopic investigation on α-difluoromethyl-ornithine (DFMO), a potential target as chemotherapeutic agent
- PS2-39**     **A. K. Przybył, Z. Nowakowska**  
A comparative study of EI-MS and NMR in analysis of the new derivatives of cytosine with aminoacids
- PS2-40**     **C. M. Muntean, R. Misselwitz and H. Welfle**  
A Raman spectroscopic study on the DNA structure at reduced pH values, in the presence of Mn<sup>2+</sup> ions
- PS2-41**     **B. Jasiewicz, K. Skrycki**  
New methyl sparteine derivatives as potential hypoglycemic agents
- PS2-42**     **P. Bruździak, J. Stangret**  
Characterization of changes in structure and stability of lysozyme caused by glycine and its methyl derivatives
- PS2-43**     **P. Rakowska, M. Olszewski, J. Stangret, J. Kur**  
The use of FT-IR spectra in examination of structure and stability changes of *Taq*SSB protein and its complex with ssDNA

- PS2-44**     **A. Panuszko, D. Wyrzykowski, J. Stangret**  
Spectroscopic, calorimetric and ab initio study of water interactions with stabilizing and denaturing osmolytes
- PS2-45**     **S. Celik, A. E. Ozel , S. Akyuz , S. Kecel and G. Agaeva**  
Conformational preferences, experiment and theoretical vibrational spectra of cyclo(Gly-Val) dipeptide
- PS2-46**     **T. Pazderka, V. Kopecký Jr., K. Hofbauerová, V. Baumruk**  
Raman and infrared spectroscopy of amino acids and its implication for improvement of the protein secondary structure determination
- PS2-47**     **S. Kecel, A. E. Ozel, S. Akyuz, S. Celik, G. Agaeva**  
Structural and spectroscopic elucidation of L-proline tyrosine (L-pro-tyr) dipeptide
- PS2-48**     **E. Kočišová, M. Procházka, J. Štěpánek**  
DCDR spectroscopy as efficient tool for study of liposome interaction with biomolecular complexes
- PS2-49**     **E-L. Karjalainen, A. Barth**  
Calculations of infrared spectra of the amide I band of proteins - method development and application to SR Ca<sup>2+</sup>-ATPase
- PS2-50**     **A. Dijanošić, S. Miljanić, Z. Meić, I. Piantanida, M. T. Albelda, A. Sornosa-Ten, E. García-Espana**  
Surface-enhanced Raman study of the interactions between cationic polyamines and polynucleotides
- PS2-51**     **Y. Akkaya , K. Balci, S. Akyuz**  
Studies on Valine-Tyrosine, antihypertensive dipeptide in aqueous solution by Raman spectroscopy
- PS2-52**     **G. Uraz, B. Çelik**  
Evaluation of Existence of Biofilm in the Isolates of Pseudomonas with Spectrophotometer
- PS2-53**     **O. Cozar, L. Szabó, I. B. Cozar, N. Leopold, V. Chiş, L. David**  
Vibrational and DFT study of some cardiovascular drugs and their copper complexes

- PS2-54**     **P. Taddei, E. Modena, A. Tinti, F. Siboni, C. Prati, M.G. Gandolfi**  
Vibrational investigation on the *in vitro* bioactivity of commercial and experimental calcium-silicate cements for root-end endodontic therapy
- PS2-55**     **I. Iriepa, J. Bellanato, E. Gálvez**  
Synthesis, conformational and pharmacological study of some carbamates derived from endo-8-methyl-8-azabicyclo[3.2.1]octan-3a-ol hydrochlorides
- PS2-56**     **V. Venuti, V. Crupi, D. Majolino, A. Mazzaglia, A. Paciaroni, R. Stancanelli**  
Chiral recognition and complexation behaviour of  $\beta$ -CyDs vs. L-, D- and DL-serine by FTIR-ATR spectroscopy.
- PS2-57**     **J. Hudecová, J. Kapitán, V. Baumruk, P. Bouř**  
Flexibility of a model cyclic hexapeptide studied by the Raman and Raman Optical Activity
- PS2-58**     **S. Osmanoglu, Y. Dicle**  
Free radicals in gamma irradiated neurological drug topimarate: an epr study

### Material and Surfaces

- PS2-59**     **S. Krehula, S. Musić**  
The influence of platinum(IV) ions on the formation of iron oxides in a highly alkaline medium
- PS2-60**     **M. Samsonowicz, E. Regulska, W. Lewandowski**  
Influence of alkaline earth metals on molecular structure of 3-nitrobenzoic acid in comparison with alkali metals effect.
- PS2-61**     **E. Regulska, M. Kalinowska, W. Lewandowski**  
Experimental and theoretical study of molecular structure of alkali metal para substituted benzoates.
- PS2-62**     **S. Kumar, A. Barth**  
Phosphoenolpyruvate and  $Mg^{2+}$  binding to pyruvate kinase monitored by infrared spectroscopy
- PS2-63**     **C. Rémazeilles, P. Refait**

FTIR-ATR analysis of synthetic iron(II-III) hydroxysalts green rusts

- PS2-64**     **E. Akalin, S. Akyuz**  
Experimental and theoretical vibrational spectroscopic investigation of Zn(II) halide complexes of pyridine derivatives
- PS2-65**     **O.Cozar, I.Bratu, L.Szabo, I.B.Cozar, M.Culea, L.David**  
IR and EPR study of copper(II) complexes with <sup>15</sup>N-labelled lysine and ornithine
- PS2-66**     **A. Bebu, A. Kozma, E. Forizs, M. Toderas, L. David**  
Spectral and ESR study of Cu(II), Co(II) and Ni(II) theophyllinato complexes containing propanolamine ligands
- PS2-67**     **A. Stanila, S. Stanila, L. Leopold**  
Spectroscopic investigations of some transitional metals complexes with methionine as ligand
- PS2-68**     **A. Baran, E. Mrozek, M. Baranska**  
FT-Raman analysis of luteolin and its complexes with Al (III)
- PS2-69**     **I. Georgieva, N. Trendafilova, I. Kostova, Tz. Mihaylov**  
FTIR, Raman, NMR and theoretical studies of lanthanide complexes with coumarin-3-carboxylic acid
- PS2-70**     **M. Kalinowska, R. Świsłocka, W. Lewandowski**  
Zn(II), Cd(II) and Hg(I) complexes of biologically important ligands: FT-IR, FT-Raman, <sup>1</sup>H and <sup>13</sup>C NMR studies
- PS2-71**     **R. Świsłocka, M. Kowczyk, M. Kalinowska, W. Lewandowski**  
Molecular structure of alkali metal salts of *p*-coumaric acid: Spectroscopic (FT-IR, FT-Raman, <sup>1</sup>H and <sup>13</sup>C NMR) and theoretical (in B3LYP/6-311++G\*\* level) studies
- PS2-72**     **P. Matejka, M. Vyskovska, A. Kokaislova, V. Prokopec, J. Cejkova, M. Clupek**  
Surface-enhanced spectroscopic methods on metal nano-surfaces: What is the role of oxidation reduction cycles?
- PS2-73**     **J.L. Castro, J.F. Arenas, M.R. López-Ramírez, J.C. Otero**  
Surface-Enhanced Raman Scattering of aromatic amides

- PS2-74**     **M. Kokoskova, M. Prochazka B. Vlckova**  
SERS/SERRS spectra and excitation profiles of Ru (II) bis(2,2-bipyridine)(4,4-dicarboxybipyridine) complex in systems with Ag nanoparticles: chemisorption versus electrostatic bonding
- PS2-75**     **M. Giloan, S. Astilean**  
Computation of electromagnetic properties of plasmonic metamaterials with relevance in SERS by using S-parameter retrieval approach
- PS2-76**     **A.M. Gabudean, S. Astilean**  
A pH-dependent SERS study of 4-aminotiophenol adsorbed on gold nanorods
- PS2-77**     **J.L. Castro, M.R. López-Ramírez, J.F. Arenas, J.C. Otero**  
SERS of benzenesulfonamide adsorbed on silver nanoclusters
- PS2-78**     **P. Šimáková, M. Procházka**  
SERRS microspectroscopy of porphyrins on Ag immobilized nanoparticles
- PS2-79**     **N. Mircescu, L. Szabo, N. Leopold, O. Cozar, V. Chi**  
Surface-enhanced Raman and DFT study on melamine
- PS2-80**     **I. López-Tocón, J.C. Otero, J.F. Arenas, J.V. Garcia-Ramos, S. Sanchez-Cortes**  
Trace-detection of triphenylene by SERS spectroscopy using functionalized silver nanoparticles with bis-acridinium lucigenine

### ***Ultrafast spectroscopy and computational methods***

- PS2-81**     **F. Muniz Miranda, M. Pagliai, G. Cardini, V. Schettino**  
Spectroscopic properties of hydrogen-bonded systems by wavelet analysis
- PS2-82**     **C. Araujo-Andrade, S. Lopes, R. Fausto, A. Gómez-Zavaglia**  
Conformational study of arbutin by quantum chemical calculations and multivariate analysis
- PS3-83**     **M. Ristova, J. Petreska, Lj. Pejov, B. Šoptrajanov**  
Conformational Equilibria and Intramolecular Proton Transfer in Hydrogenmalonate Anion: Influence of the Crystalline Environment. A

## Combined Vibrational Spectroscopic and Quantum Chemical Study

- PS2-84**     **H. Yurtseven, B. Raşitoğlu**  
Vibrational frequencies studies as a function of pressure near the I-II phase transition in solid benzene
- PS2-85**     **H. Yurtseven**  
Critical behavior of the order parameter from birefringence and Raman intensity data close to the  $\lambda$ -transition in  $\text{NH}_4\text{Br}$
- PS2-86**     **N. Trendafilova, I. Georgieva, B.S.Creaven**  
Structure and spectroscopic properties of Ni(II), Co(II) and Zn(II) complexes with coumarin derivative predicted by DFT calculations
- PS2-87**     **C. D. Contreras, A. E. Ledesma, J. Zinzuk, S. A. Brandán**  
Structural and vibrational study of 2-benzyl-4,5-dihydro-1*H*-imidazole
- PS2-88**     **E. C. Aguiar, J. B. P. da Silva, M. N. Ramos**  
A theoretical interpretation of the Infrared intensities of Maleimide
- PS2-89**     **G. Keresztury, T. Sundius, M. Rogojerov, Cs. Németh**  
Performance of polarized continuum solvation models in DFT prediction of IR band polarization properties for anisotropic LC solutions
- PS2-90**     **A. Padilla, J. Pérez**  
A simulation study of the far-infrared absorption spectra of HCl diluted in liquid Ar
- PS2-91**     **A. Milani, F. Innocenti, C. Castiglioni**  
Raman spectra of polyyenes and cumulenes: a computational investigation
- PS2-92**     **L. C. Bichara, E. G. Ferrer, H. E. Lanús, C. G. Nieto, S. A. Brandán**  
Theoretical and experimental vibrational study of anhydrous Citric Acid as monomer and dimer
- PS2-93**     **T. Teslaru, A. Sebi, R. Stanculescu, D.-O. Dorohoi**  
Spectral and quantum -chemical characterization of some carbanion monosubstituted cycloimmonium Ylids
- PS2-94**     **R.-E. Stanculescu, V. Sunel, D.-O. Dorohoi**  
Electro-optical parameters of some thiosemicarbazides studies by

spectral and computational means

- PS2-95** N. F.C. Mendes, **P. Ribeiro-Claro**  
Crystal polymorphism: a combined approach using vibrational spectroscopy and ab initio calculations
- PS2-96** **O.V.Postylyakov**  
Transformation of spectral radiance by inelastic and elastic scattering in the gaseous atmosphere
- PS2-97** M. Avadanei, **Virgil Barboiu**, **Mihaela Dulcescu**, **Lenuta Profire**, **Dana-Ortansa Dorohoi**  
7-[2-Hydroxy-3(-4-Acetyl-Amino)-Phenoxy-Propyl]-1,3 Dimethylxantine derivatives characterized by hyperchem 8.0.6 and spectral means
- PS2-98** R.M. Mahfouz, **N.S.Al-Hokbany**, **S.M.Akriche**, **M.Rzaigui**  
Structural and theoretical studies of 2-amino-3-nitropyridine
- PS2-99** C. Gellini, **M. Muniz-Miranda**, **P. R. Salvi**, **M. Alloisio**, **G. Dellepiane**  
Structural and vibrational properties of photochromic polydiacetylenes
- PS2-100** **D. Duce**, M. Ottonelli, **M. Piccardo**, **G. Dellepiane**  
A theoretical study on the spectroscopical effects of rhodamine b and noble metals nanoparticles interactions
- PS2-101** M. Pagliai, **F. Muniz Miranda**, **G. Cardini**, **R. Righini**, **V. Schettino**  
Hydrogen bond dynamics of methyl acetate in methanol
- PS2-102** **T. A. Ford**  
*Ab initio* studies of the homodimers of methane and silane, and of methyl and silylfluoride and chloride
- PS2-103** **G. Świdorski**, **S. Wojtulewski**, M. Kalinowska, **R. Świśtocka**, **W. Lewandowski**  
Effect of alkali metal ions on the pyrrole and pyridine  $\pi$ -electron systems in pyrrole-2-carboxylate and pyridine-2-carboxylate molecules: : FT-IR, FT-Raman, NMR and theoretical studies
- PS2-104** M. J. Wójcik, **J. Kwiendacz**, **M. Boczar**, **Ł. Boda**, **Y. Ozaki**  
Theoretical and spectroscopic study of hydrogen bond vibrations in

imidazole and its deuterated derivative

- PS2-105** **G. Mile, M. Oltean, V. Chis**  
Potential energy curves for PTCDI and PTCDA dimers obtained by MP2 and DFT methods with dispersion correction
- PS2-106** **M. Candelaresi, L. Bussotti, M. Paolantoni, P. Foggi**  
Methanol under moderate pressures: a dynamical study by femtosecond transient spectroscopy
- PS2-107** **E. Collini, F. Todescato, C. Ferrante, R. Bozio**  
Energy Transfer across metal films mediated by Surface Plasmon Polaritons: a time-resolved fluorescence study
- PS2-108** **B. Brożek-Płuska, P. Ciąćka and H. Abramczyk**  
Vibrational dynamics at the phospholipid - water interface
- PS2-109** **T. Atsbeha, L. Bussotti, A. Marcelli, P. Foggi, S. Cicchi, G. Ghini, P. Fabbrizi**  
Photophysical characterization of low molecular weight organogels for energy transfer and light harvesting
- PS2-110** **A. Lapini, P. Tourón Touceda, S. Mosquera Vazquez, M. Lima, A. Dei, P. Foggi, R. Righini**  
Characterization of a cobalt-dioxolene complex by Transient Infrared Spectroscopy
- PS2-111** **S. Mosquera Vazquez, P. Foggi, A. Lapini, P. Tourón Touceda, A. Abbotto, F. De Angelis, M. Lobello**  
Transient absorption spectroscopy of Heteroaromatic Donor-Acceptor  $\pi$ -conjugated 2,2'-Bipyridines
- PS1-112** **M. Lima, A. Lapini, P. Tourón Touceda, S. Mosquera Vazquez**  
Cross Phase modulation in visible-pump/infrared-probe spectroscopy

### ***Vibrational and electronic spectroscopy***

- PS2-113** **R. M. Pinto, A. A. Dias, M. L. Costa**  
Study of tetrazole derivatives by UV photoelectron spectroscopy and outer-valence Green's function methods.
- PS2-114** **R. M. Pinto, G. Copeland, A. A. Dias, M. L. Costa, J. M. Dyke**

Thermal decomposition of benzyl azide and its methyl derivatives studied by UV photoelectron spectroscopy and theoretical calculations.

- PS2-115** **W. Sasiadek, E. Kucharska, I. Bryndal, M. Wandas, J. Hanuza**  
Excited electronic states, crystal structure and DFT quantum chemical calculations of 2-amino-4-methyl-3-nitropyridine.
- PS2-116** **D. O. Dorohoi, A. Airinei, R. I. Tigoianu**  
Revisiting the electronic spectra of anthracene.
- PS2-117** **M. Scholz, R. Džedić, A. Svoboda, J. Hála**  
TPP and singlet Oxygen quenching by Carotene in solution.
- PS2-118** **J. Polak, M. Bartoszek, M. Żądło, W.W. Sułkowski**  
The EPR study of humic acid extracted from sediment collected at various seasons.
- PS2-119** **T. Iwata, Y. Mizutani**  
Comparison of a Pulsed-Excitation and a Phase-Modulation Method for estimating fluorescence lifetimes using a Convolved-Autoregressive Model and a high-gain PMT.
- PS2-120** **A. Mezzetti, S. Protti, J.-P. Cornard, C. Lapouge, A. Idrissi, M. Fagnoni, A. Albini**  
Solvent effects on 3-hydroxyflavone photophysics / photochemistry. Relevance to its application in optical devices and its use as a (bio-)sensor.
- PS2-121** **A. Mezzetti, S. Protti, S. Lazzaroni, A. Barras, N. Montfillette-Dupont, C. Lapouge, J.P. Cornard**  
Spectroscopic investigation of flavonoids of biomedical relevance in solution and inside lipid nanocapsules.
- PS2-122** **D. Cheshmedzhieva, B. Hadjieva, S. Ilieva, D. Nalbantova, B. Galabov.**  
Reactivity of carbamates in the alkaline hydrolysis reaction.
- PS2-123** **L. Grisanti, C. Sissa, F. Terenziani, A. Painelli**  
CT chromophores and complexes: Spectra and models.
- PS2-124** **G. Piani, M. Pasquini, G. Pietraperzia, E. M. Castellucci, M.**

**Becucci**

Different methods for ionization threshold determination.

- PS2-125** M. Scotoni, A. Mazzalai  
Velocity dependence of C<sub>2</sub>H<sub>2</sub> rotational temperature in a supersonic expansion.
- PS2-126** M. Becucci, G. Ferrari, M. Prevedelli, I. Boscolo, F. Castelli, S. Cialdi, F. Villa, M.G. Giammarchi  
A laser system for efficient excitation of positronium towards Rydberg levels.
- PS2-127** B. M. Giuliano, V. Feyer, K.C. Prince, M. Coreno, L. Evangelisti, S. Melandri, W. Caminati  
Tautomerism in pyrimidine derivatives investigated with core level spectroscopy techniques
- PS2-128** S. Abbruzzetti, A. Bonamore, A. Boffi, A. Feis, P. Foggi, C. Gellini, A. Marcelli, P.R. Salvi, C. Viappiani  
Time-resolved spectroscopy of native and mutated *Thermobifida fusca* hemoglobins
- PS2-129** M. Ceppatelli, R. Bini, V. Schettino  
High pressure photoinduced reactivity in clathrate hydrates
- PS2-130** G. Das, M.L. Coluccio, A. Nicastrì, F. Gentile, F. De Angelis, E. Di Fabrizio, G. Cuda  
Raman spectroscopy for the evaluation of structural changes of peptides

**GISR**

- PS2-131** G. Compagnini, G. Forte, F. Giannazzo, V. Raineri, A. La Magna, I. Deretzis  
Ion beam induced defects in graphene: Raman spectroscopy and DFT calculations
- PS2-132** C. Lofrumento, M. Ricci, L. Bachechi, D. De Feo, E. M. Castellucci  
Spectroscopic analyses on rock art paintings from east central Ethiopia.

- PS2-133 **M. P. Marzocchi, A. Belshi**  
Combined analysis of structural and spectral observables for heme proteins.
- PS2-134 **F.P. Nicoletti, E. Droghetti, A. Feis, A. Boffi, G. Smulevich**  
Resonance Raman and UV-vis absorption spectra of *Thermobifida fusca* truncated hemoglobin in its ferric state.
- PS2-135 **F. Palombo, P. Sassi, M. Paolantoni, A. Morresi, M. G. Giorgini**  
Raman spectroscopic study of the effects of ion solvation on liquid phase structure and dynamics of LiI-acetone solutions.
- PS2-136 **G. Piani, L. Rubio Lago, M. Becucci**  
Photoelectron imaging on Iodine atoms produced by CF<sub>3</sub>I photodissociation.
- PS2-137 **M. Biczysko**  
Computational spectroscopy as a tool to interpret experimental results: from small molecules in the gas phase to large systems in condensed phases
- PS2-138 **A. Weselucha-Birczyńska, L. Natkaniec-Nowak**  
Raman microspectroscopic study of organic inclusions in „watermelon” tourmaline from the Paprok mine (Nuristan, Afganistan)
- PS2-139 **C. Paluszkiwicz, A. Weselucha-Birczynska, E. Stodolak**  
Raman Spectroscopy Investigations of a Chitosan-Clay Nanocomposite

13.30 - 15.00 lunch

## AFTERNOON SESSION at Centro Didattico Morgagni

### ORAL PRESENTATIONS

- Room 101** ***Ultrafast spectroscopy and computational methods***  
15.00 - 15.20 **A.A. Bakulin, J.C. Hummelen, P.H.M. van Loosdrecht, M.S. Pshenichnikov**  
30-fs Hole-transfer dynamics in polymer/PCBM bulk heterojunction

- 15.20 - 15.40 **T. Maňal, F. Šanda, N. Christensson, V. Butkus, J. Olšina, V. Balevicius Jr., L. Valkunas**  
Two-dimensional coherent electronic spectroscopy of electron-phonon coupling
- 15.40 - 16.00 **S.V. Krasnoshchekov, E.V. Isayeva, N.F. Stepanov**  
Mixed numerical/analytic solution of the anharmonic vibrational problem for a polyatomic molecule using high orders of canonical perturbation theory
- 16.00 - 16.20 **M.J. Wójcik, Ł. Boda, M. Boczar**  
Theoretical study of proton tunneling in the excited state of tropolone

**Room 107** *Young Scientists*

- 15.00 - 15.20 **C. F. Dascalu, B. C. Zelinschi, D. O. Dorohoi**  
Main refractive indices of some carpathian crystals
- 15.20 - 15.40 **M. Vyskovska, V. Prokopec, M. Clupek, A. Kokaislova, J. Cejkova, P. Matejka**  
Development of copper nanostructured materials for surface-enhanced Raman scattering spectroscopy
- 15.40 - 16.00 **R. E. Stanculescu, V. Sunel, D. O. Dorohoi**  
electro-optical parameters of some thio-semicarbazides studied by spectral and computational means
- 16.00 - 16.20 **F. Palombo, P. Sassi, M. Paolantoni, A. Morresi, M. G. Giorgini**  
Raman spectroscopic study of the effects of ion solvation on liquid phase structure and dynamics of LiI-acetone solutions

**Room 108** *Vibrational and electronic spectroscopy*

- 15.00 - 15.20 **V. Aleksa, J. Kausteklis, Z. Gdaniec, V. Balevicius**  
2D Raman correlation and NMR spectroscopy study of liquid crystalline ionogel phase formation in ionic liquid/H<sub>2</sub>O mixtures
- 15.20 - 15.40 **S. Cîntă Pînzaru, A. Falamas, N. Leopold, C. Dehelean, C. Lehene**  
Challenging SERS from biomolecules to tissue
- 15.40 - 16.00 **J. Grdadolnik**  
Backbone structures of 19 dipeptides in Aqueous Solution
- 16.00 - 16.20 **Horiba Jobin-Yvon**  
Advances in Raman spectroscopy

**Room 109** *GISR*

- 15.00 - 15.20 **B. Rossi, G. Cazzolli, G. Vilianni, C. M.C. Gambi, S. Marchetti**

Molecular aggregation processes in self-assembled micellar systems investigated by Raman scattering and numerical simulation

15.20 - 15.40 **E. Fazio, F. Neri, S. Trusso**

Surface-enhanced Raman scattering (SERS) from SnO<sub>2</sub> material

15.40 - 16.00 **G. D'Avino, A. Girlando, M. Masino, A. Painelli**

Electron-phonon entanglement near a ferroelectric phase transition: evidences from low-frequency Raman scattering

16.00 - 16.20 **M.A. Ferrara, L. Sirleto, I. Rendina, S.N. Basu, J. Warga, R. Li, L. Dal Negro**

Enhanced stimulated Raman scattering in silicon nanocrystals embedded in silicon-rich nitride/silicon superlattice structures

16.20 - 16.50 **coffee break**

**Room 101** *Ultrafast spectroscopy and computational methods*

16.50 - 17.10 **K. Itoh**

DFT calculation of low frequency vibrational modes of polypeptides consisting of L- and D-Alanine residues

17.10 - 17.30 **T. Burova, A. Anashkin**

Quantum-mechanical analysis of intensity distribution in resonance hyper Raman spectra of polyatomic molecules

17.30 - 17.50 **A. Milani, C. Castiglioni**

Atomic charges and charge fluxes derived from IR intensities

17.50 - 18.10 **V.H. Rusu, M.N. Ramos, R.L. Longo**

CCFOM and CCFDF models to interpret infrared intensities: A comparative study

**Room 107** *Young Scientists*

16.50 - 17.10 **S. Kumar, A. Barth**

Phosphoenolpyruvate and Mg<sup>2+</sup> binding to pyruvate kinase monitored by infrared spectroscopy

17.10 - 17.30 **V. Andrushchenko, H. Wieser, M. Straka, P. Bouř**

Combination of circular dichroism spectroscopy with theoretical spectra simulations as a tool for structural studies of macromolecules

17.30 - 17.50 **N. O. B. Lüttschwager, T. N. Wassermann, S. Coussan, M. A. Suhm**

Environmental and vibrational influence on the proton transfer in malonaldehyde

**Room 108** *Vibrational and electronic spectroscopy*

- 16.50 - 17.10 **V.A. Karachevtsev, A.M. Plokhotnichenko, M.V. Karachevtsev and V. S. Leontiev**  
Noncovalent interaction of carbon nanotubes with DNA and polynucleotides: UV absorption spectroscopy and molecular dynamic simulation
- 17.10 - 17.30 **M. Kozanecki, P. Zawadzka, R. Kisiel, M. Pastorczak**  
Intermolecular interactions in water-aliphatic halogen systems - vibrational spectroscopy studies
- 17.30 - 17.50 **B. Řezáčová, Ch. Zentz, P-Y Turpin, J. Štěpánek**  
Spectroscopic study of MADS box and its interaction with DNA
- 17.50 - 18.10 **V. Kopecký Jr., K. Hofbauerová, J. Kohoutová, J. Štěpánek, R. Ettrich**  
Can drop coating deposition Raman spectroscopy distinguish shortcomings or inaccuracies in protein crystals?

**Room 109 GISR**

- 16.50 - 17.10 **M. Paolantoni, L. Comez, D. Fioretto, M. E. Gallina, L. Lupi, A. Morresi, S. Perticaroli, P. Sassi, F. Scarponi**  
The dynamics of water in aqueous solutions of biological molecules assessed by broadband depolarized light scattering experiments
- 17.10 - 17.30 **B.D. Howes, D. Giordano, L. Boechi, M. Fittipaldi, D.A. Estrin, M. Coletta, G. Di Prisco, C. Verde, G. Smulevich**  
The pronounced structural flexibility of the 2/2 hemoglobin of the antarctic cold-adapted *Pseudoalteromonas haloplanktis* TAC125
- 17.30 - 17.50 **M. Tommasini, A. Lucotti, G. Zerbi**  
A Raman study of Schiff base protonation in bacteriorhodopsin and related molecular models
- 17.50 - 18.10 **P. Sassi, G. Onori, A. Giugliarelli, M. Paolantoni, S. Cinelli, A. Morresi**  
The thermal unfolding of lysozyme in solution: the role of the solvent

**20.30 CONFERENCE DINNER at Palazzo Borghese**

**Friday, September 3****MORNING SESSION****INVITED LECTURES Room 101 & 109 (109 videoconference)**

9.00 - 9.45

**R. J. Hemley**

Molecules under pressure

9.45 - 10.30

**M. Parrinello***Title*10.30 - 11.00 **coffee break**

11.00 - 11.45

**V. Balzani**

Photochemically controlled molecular devices and machines

11.45 - 12.00

**S. Astilean, M. Baia, D. Maniu, C. Farcau, M. Iosin, V. Canpean, S. Boca, M. Potara, A. M. Gabudean**

New approaches to develop multifunctional plasmonic nanosensors for bioanalytical applications

12.00 - 12.30

**S. Astilean**

EUCMOS 2012 presentation

12.30 - 12.45

**Final remarks**