

## Thursday 28. 8. 2014

- 9:00 – 9:45 **HS 3A** Plenary Talk P6: Hugh Burrows *Transient absorption spectra and theoretical studies of excited and charged states of organic materials for optoelectronics*
- 9:45 – 10:30 **HS 3A** Plenary Talk P7: Pavel Hobza *Noncovalent interactions: theory and applications*
- 10:30 – 11:00 Coffee Break
- 11:00 – 13:00** **HS 3A Session 15 Raman Spectroscopy**
- 11:00 – 11:20 M. Kozanecki, M.N. Olejniczak *Intermolecular Interactions in Hydrogel-NSAIDS Systems – Raman Spectroscopy Studies*
- 11:20 – 11:40 Dmytro Solonenko, Alexander Milekhin, Martin Panholzer, Kurt Hingerl, Ovidiu D. Gordan, Dietrich R.T. Zahn *Interference Enhanced Raman Scattering of F<sub>16</sub>CuPc Films*
- 11:40 – 12:00 Paola Sassi, Silvia Corezzi, Stefania Perticaroli, Lucia Comez, Alessandra Giugliarelli, Marco Paolantoni, Daniele Fioretto and Assunta Morresi *Low Frequency Vibrations of Native and Denaturated Lysozyme: A Raman Study*
- 12:00 – 12:20 P. Filipczak, M. Wadlewska, M. Kozanecki *Influence of Selected Inorganic Salts on Raman Resonance Phenomenon in Water*
- 12:20 – 12:40 E.A. Sagitova, P. Donfack, K.A. Prokhorov, G.Yu. Nikolaeva, P.P. Pashinin, N.D. Merekalova, V.A. Gerasin, and A. Materny *The Symmetric C-C Stretching Mode Splitting in Raman spectra of substances, containing alkylammonium ions*
- 12:40 – 13:00 K.A. Prokhorov, Yu.V. Zavgorodnev, G.Yu. Nikolaeva, E.A. Sagitova, T.V. Vlasova, P.P. Pashinin, T.M. Ushakova, L.A. Novokshonova, E.E. Starchak, P.M. Nedorezova, A.N. Klyamkina, P. Donfack, A. Materny *Raman Diagnostics of Copolymers and Polymer Blends*
- 11:00 – 13:00** **HS 3B Session 16 Spectroscopy of Polymers and Films**
- 11:00 – 11:20 Cosutchi Irina Andreea, Dimitriu Dan Gheorghe, Zelinschi Carmen Beatrice, Breaban Iuliana and Dorohoi Dana Ortansa *Optical Activity of Transparent Polymer Foils Characterized by Spectral Means*
- 11:20 – 11:40 Stefano Radice, Alberto Milani, Chiara Castiglioni *Tetrafluoroethylene Based Polymers; Spectroscopy Studies and Quantum Chemical Modeling*
- 11:40 – 12:00 Dr. Gernot Höhne, Dr. Mathias Boese, Eric Klein *Automated FTIR Microscopy in the Polymer Industry*
- 12:00 – 12:20 Mario Krieg and Hans Bettermann *Tracking of micellization by fluorescence spectroscopy*
- 11:00 – 13:00** **HS 3C Session 17 Methods II**
- 11:00 – 11:20 A. Kraus, R. Gröble, S. Mirz *Precise and Accurate Transmission Spectra Computed by a Modified Data Analysis Procedure in FTIR Spectrometry*

## Overview

- 11:20 – 11:40 R. Größle, A. Kraus and S. Mirz *Non Linear Effects in IR Absorption Spectroscopy of Liquid Hydrogen Isotopologues*
- 11:40 – 12:00 Martin Labus, Hans Bettermann *Online In-Situ Raman Studies of Processes in a High Temperature PEM Fuel Cell*
- 12:00 – 12:20 H. Yurtseven and H. Özdemir *Calculation of the Specific Heat Using the Raman Frequency Shifts for the Solid I-II Transition in Benzene*
- 12:20 – 12:40 S. Mirz, R. Größle, A. Kraus *Investigation of the Influence of ortho/para Conversion on the Infrared Spectra of Liquid Hydrogen and Deuterium*
- 12:40 – 13:00 Sanjay Kumar *Comparative Study of Excited State Dipole Moment of Coumarin Laser Dyes: Solvent and Substituent Effect*
- 13:00 – 14:30 Lunch
- 14:50 – 16:30** ***HS 3A Session 18 Dynamics and Time Resolved Spectroscopy II***
- 14:50 – 15:10 A. Mezzetti, E.Kish Perrin, R. Spezia, M. Mendes-Pinto, D. Bovi, L. Guidoni, M. Basire, R. Vuilleumier, B. Robert *Solute-Solvent and Pigment-Protein Interactions in Carotenoids. A Combined Resonance Raman, Time-Resolved FTIR and QM/MM Study of Peridinin*
- 15:10 – 15:30 T. Villnow, G. Ryseck, R. Mundt, S. Fröbel and P. Gilch *Thioxanthone – A Photophysical Chimera*
- 15:30 – 15:50 Glushkov Alexander, Kondratenko P.A., Svinarenko Andrey, and Sakun Tat'yana *Spectroscopy of Cooperative Laser Electron- $\gamma$ -Nuclear Processes in Diatomic, Multiatomic Molecules and Clusters*
- 15:50 – 16:10 G. M. Greetham, I. P. Clark, D. Weidmann, M. N. R. Ashfold, A. J. Orr-Ewing and M. Towrie *Waveguide Enhanced 2D-IR Spectroscopy in the Gas-Phase*
- 16:10 – 16:30 Marek J. Wojcik *Dynamics of protons in hydrogen bonds studied by theoretical methods and vibrational spectroscopy*
- 14:50 – 16:30** ***HS 3B Session 19 New Materials III***
- 14:50 – 15:10 M.N. Olejniczak, K. Piechocki, W. Kwiecinski, S. Kadlubowski and M. Kozanecki *Molecular Approach to a Role of NSAIDS in Changes of Volume Phase Transition Temperature in Thermo-Responsive Hydrogels*
- 15:10 – 15:30 A.A. Maksimova, M.I. Oshtrakh, E.V. Petrova, V.I. Grokhovsky and V.A. Semionkin *Comparative Study of Chelyabinsk LL5 Meteorite Fragments with Light and Mixed Light and Dark Lithology Using Mössbauer Spectroscopy*
- 15:30 – 15:50 P. Matějka and A. Pospíšil *Development of vibrational spectroscopic methods for analysis of cocrystals: What is the Information about Interactions of cofomers with the active ingredient?*
- 15:50 – 16:10 N.D. Curmei, G.V. Klishevich, V.I. Melnik, A.G. Tereshchenko *Significance of symmetry in the formation of impurity centers in molecular crystals*
- 16:30 – 18:00 Poster Session II
- 20:00 – 23:00 Conference Dinner