



Locations:

Registration will be held in the

Centre of the Regional Committee of Hungarian Academy of Sciences
(Jurisics Miklós str. 44., H-7624 Pécs, Hungary, Coordinates: N:46.082765, E:18.210260)

Oral presentations will be held in the

2nd floor, Lecture Hall of the Centre of the Regional Committee of Hungarian Academy of Sciences

Lunches and the Welcome Party will be held in the

3rd floor, Dining Rooms of the Centre of the Regional Committee of Hungarian Academy of Sciences

PROGRAM

4. March 2013.

16:00- Registration

19:00 Welcome Party

5. March 2013.

09:00 - 09:20 Opening Prologue

György Kosztolányi, president

Regional Committee of Hungarian Academy of Sciences

Ferenc Joó, president

Section of Chemical Sciences of the Hungarian Academy of Sciences

József Deli, president

Section of Chemical Sciences,

Regional Committee of the Hungarian Academy of Sciences

Ruth Geiger, sales and marketing Director

HORIBA Jobin Yvon

Koichi Iwata, conference co-chair

Gakushuin University, Tokyo, Japan

Sándor Kunsági-Máté, conference chair

University of Pécs, Pécs, Hungary

Performance of the string-quartet of the Institute of Music, Faculty of Music and Visual Arts, University of Pécs

Márta Flóra Kovács - violin

Zsuzsanna Hidvégi - viola

Gergely Erdei - violin

Tamás Kirkósa - violoncello

09:20 – 09:30 Technical Break

1st Session: Weak Molecular Interactions: Examples in General View

Session Chair: Walter M.F. Fabian

- 09:30 – 10:15 Takayuki Ebata (*Hiroshima University, Japan*)
Structure and photo-physics of host-guest complexes
and bio-related molecules in the gas phase
- 10:15 – 10:30 Coffee Break
- 10:30 – 11:15 Barbara Kirchner (*University of Bonn, Germany*)
Associated liquids from unconventional methods: Quantum cluster theory
and floating orbital molecular dynamics
- 11:15 – 11:45 Miklós Kubinyi (*Research Centre of Natural Sciences,
Hungarian Academy of Sciences, Hungary*)
Synthetic fluorescent sensors for recognition of nucleotides
- 11:45 – 13:15 Lunch

2nd Session: Raman as Fruitful Tool in Research of Weak Molecular Interactions

Session Chairs: Ruth Geiger and Takayuki Ebata

- 13:15 – 13:30 Ruth Geiger (*HORIBA Jobin Yvon, France*)
Evolution of Raman Instrumentation Driven by Available Technologies
- 13:30 – 14:15 Tatsuyuki Yamamoto (*Shimane University, Japan*)
The application of Raman spectroscopy on the biological tissues and
living cells
- 14:15 – 14:35 Konstantinos Andrikopoulos (*Foundation for Research and Technology-
Hellas, Greece*)
Influence of silver nano-particles agglomeration kinetics
on the Surface enhanced Raman signal
- 14:35 – 14:50 Coffee Break
- 14:50 – 15:35 Sophie Lecomte (*CNRS-University of Bordeaux, France*)
Surface Enhanced Raman Scattering in Microfluidics Devices to detect
biomolecules
- 15:35 – 15:45 Romain Bruder (*HORIBA Jobin Yvon, France*)
From fundamental studies to probing approaches:
Raman spectroscopy to investigate and detect weak molecular interactions
- 15:45 – 16:00 Peter Vernhout (*AIST Nano Technologies International, Netherlands*)
Atomic Force Microscopy, Technologies and Products
- 16:00 – 16:45 Poster Session

3rd Session: Pécs: Science – Culture – History

Session Chair: László Kollár and Sándor Kunsági-Máté

- 16:45 – 17:15 Transfer to the Szentágotthai Research Center
- 17:15 – 17:35 Zsuzsanna Helyes (*scientific secretary, Szentágotthai Research Center*)
Scientific portfolio of the Szentágotthai Research Center
- 17:35 – 17:45 The structure of the building of the Research Center (film)
- 17:45 – 18:00 Sparks: Hungarian Creativity and Innovation (film)
- 18:00 – 18:30 Transfer to the City Center, walk to the Mayor's Office of Pécs
- 18:30 – 19:00 Mayor's salutation
Presentation about the History of Pécs
- 19:00 – 22:00 Conference Dinner

6. March 2013.

4th Session: Theoretical Investigations of Weak Molecular Interactions

Session Chair: Barbara Kirchner

- 09:00 – 09:45 Walter M.F. Fabian (*Karl Franzens Universität, Austria*)
Noncovalent interactions: wave function vs. density functional based methods
- 09:45 – 10:05 Joachim Friedrich (*Technical University Chemnitz, Germany*)
Highly Accurate Electronic Structure Methods for Weak Interactions
- 10:05 – 10:25 Tobias Risthaus (*University of Bonn, Germany*)
Comparison of DFT-based Treatments of Dispersion Interactions
in Supramolecular Complexes
- 10:25 – 10:40 Coffee Break
- 10:40 – 11:25 Anne-Marie Kelterer (*Graz University of Technology, Austria*)
Weak interactions in the excited state
- 11:25 – 11:45 Oldamur Hollóczki (*University of Bonn, Germany*)
Carbon Dioxide in Ionic Liquids: Solvation, Ionic Liquid Effect,
Carbene Formation
- 11:45 – 12:05 Gergely Matisz (*University of Pécs, Hungary*)
Structure of Neat and Binary Hydrogen-bonded Liquids of
Primary Alcohols within the Quantum Cluster Equilibrium Theory
- 12:05 – 12:25 János Ángyán (*Université de Lorraine & CNRS, France*)
Range-separated hybrid density functional methods with many-body
corrections for modelling intermolecular interactions
- 12:25 – 13:20 Lunch

5th Session: Weak Molecular Interactions in Biology

Session Chairs: Anne-Marie Kelterer and Sophie Lecomte

- 13:20 – 13:40 Radu Silaghi-Dumitrescu (*Babes-Bolyai University, Romania*)
Weak interactions dictating secondary and tertiary structure in proteins
- 13:40 – 14:00 Zsolt Valicsek (*Pannon University, Hungary*)
Possibility and applicability of aggregation of porphyrins
- 14:00 – 14:20 Miklós Poór (*University of Pécs, Hungary*)
Interaction of Ochratoxin A with alkaline earth ions
- 14:20 – 14:40 Koichi Iwata (*Gakushuin University, Japan*)
Examination of Solution Phase Partial Orders Formed
with Weak Molecular Interactions. Time-resolved Spectroscopic Studies
- 14:40 – 14:50 Closing Remarks
- 15:00 – 18:00 Guided Tour in Pécs
- 18:00 – 19:30 Dinner
- 20:00 – 21:00 Concert in the Basilica of Pécs

Programme:

W.A.Mozart: Sancta Maria K.273
Missa brevis in B-flat major, K.275
Laudate Dominum K.339
Alma Dei Creatoris K.277

T.Albinoni: Adagio
F.Schubert: Mile cherubini in coro
J.S.Bach: Toccata and Fugue in D minor, BWV.565

The Mozart Choir and Orchestra of Basilica in Pécs

Ágnes Kuti – Soprano *Bernadett Rózsa - Alto*
József Benke – Tenor *Csaba Békési-M. – Bass*

Conductor and contributor: Szabolcs Szamosi - organ

Posters:

- P-1 F. Benz, N. Dannehl, Y. Weng, M. Yang, H.P. Strunk:
RARE EARTH LUMINESCENCE CENTERS IN SEMICONDUCTOR MATRICES –
CAN THEY BE CONSIDERED AS MOLECULAR ENTITIES?
- P-2 H.Li, J.C. Nie, S. Kunsági-Máté:
ETHANOL ASSISTED FORMATION OF FEW LAYER GRAPHENE
- P-3 J. G. Brandenburg, S. Grimme:
A GEOMETRICAL CORRECTION FOR THE INTER- AND INTRA-MOLECULAR
BASIS SET SUPERPOSITION ERROR IN HARTREE-FOCK AND DENSITY
FUNCTIONAL THEORY CALCULATIONS FOR PERIODIC SYSTEMS
- P-4 R. Sure, S. Grimme:
THERMOCHEMISTRY OF SUPRAMOLECULAR COMPLEXES USING DFT-D3 AND
HF/MINIMAL BASIS SET APPROACHES
- P-5 L. Könczöl, E. Makkos, D. Bourissou, D. Szieberth:
UNUSUAL MAIN GROUP η^2 -H₂ COMPLEXES
- P-6 Z. Kelemen, L. Nyulászi:
INVESTIGATION OF THE MECHANISM OF A CARBEN-CATALYZED
REDOXREACTION
- P-7 É. Pósfai, I. Marton, Z. Borbényi, M. Széll, Zs. László:
IDENTIFICATION OF MPL-W515L -W515K - W515R -W515A -
S505N MUTATIONS IN THROMBOPOIETIN RECEPTOR OF ESSENTIAL
THROMBOCYTHEMIA PATIENTS
- P-8 Y. Li, Z. Czibulya, M. Poór, S. Lecomte, L. Kiss, E. Harte, T. Kőszegi, S. Kunsági-Máté:
EFFECT OF ETHANOL ON THE INTERACTION OF OCHRATOXIN A WITH
HUMAN SERUM ALBUMIN
- P-9 I. Hegedüs, E. Nagy:
STABILIZATION OF β -XILOSIDASE WITH ITS QUATERNARY STRUCTURES AS
ENZYME NANOCAPSULES
- P-10 Z. Valicsek, M.P. Kiss, G. Eller, C. Szentgyörgyi, O. Horváth:
OLIGOMERIZATION OF WATER-SOLUBLE LANTHANIDE PORPHYRINS
- P-11 Zs. Kun, E. Forizs:
EXPERIMENTAL AND THEORETICAL INVESTIGATION OF CRYSTAL PACKING
INTERACTIONS IN Pd(II) AND Zn(II) THEOPHYLLYNE DERIVED COMPLEXES
- P-12 Y. Li, P. Huszthy, I. Móczár, B. Szemenyei, S. Kunsági-Máté:
PERMITTIVITY-DEPEDENT COMPLEXATIONS OF A CROWN ETHER
DERIVATIVE WITH NA⁺ AND K⁺
- P-13 Y. Li, Zs. Csók, G. Matisz, L. Kiss, L. Kollár, S. Kunsági-Máté:
A NOVEL DEEPENED CAVITAND FLUORESCENT CHEMOSENSOR FOR
DETECTION OF FE³⁺ AND CU²⁺

- P-14 Zs. Czibulya, M. P. Nikfardam, L. Kollár, S. Kunsági-Máté:
THE EFFECT OF TEMPERATURE ON THE COLOR OF RED WINE
- P-15 Zs. Czibulya, N. Mike, M. Pesti, S. Kunsági-Máté:
INTERACTION BETWEEN ZEARALENONE AND GLUTATHIONE
- P-16 Zs. Czibulya, E. Lempel, S. Kunsági-Máté:
THE APPLICATION OF RAMAN SPECTROSCOPY IN THE INVESTIGATION OF
DENTAL COMPOSITES
- P-17 B. Peles-Lemli, D. Kánnár, J.C. Nie, H. Li, S. Kunsági-Máté:
THE ADSORPTION OF ALKALI METAL IONS ONTO THE GRAPHENE SURFACE
UNDER THE EFFECT OF EXTERNAL ELECTRIC FIELD
- P-18 B. Peles-Lemli, E. Mező, D. Kánnár, L. Kollár, S. Kunsági-Máté:
DYNAMIC STRUCTURAL PROPERTIES OF THE MIXTURE OF IMIDAZOLIUM
BASED IONIC LIQUIDS AND PRIMARY ALCOHOLS
- P-19 K. Szabó, P. Wang, B. Peles-Lemli, Y. Fang, L. Kollár, S. Kunsági-Máté:
INTERACTION BETWEEN HYDROTROPIC P-TOLUENE SULFONATE AND
HYDROXYACETOPHENONE ISOMERS
- P-20 D. Kánnár, B. Peles-Lemli, L. Kollár, S. Kunsági-Máté:
EXPERIMENTAL AND THEORETICAL INVESTIGATION OF THE INTERACTION
BETWEEN ANTHRACENE-BASED MOLECULAR TWEEZERS AND CARBON
NANOTUBES