



# EDS: 2022

## Hanseatic Workshop on "Exciton Dynamics and Spectroscopy"

### CONFERENCE PROGRAMME

Center for Physical Sciences and Technology (FTMC), Vilnius, Lithuania  
Venue: FTMC at Sunrise Valley, Sauletekio Ave. 3, Vilnius, Lithuania

24 August		
8:00-9:15		REGISTRATION
9:00		CONFERENCE OPENING CEREMONY
9:00-10:30		<b>Section 1: Exciton Dynamics and Spectroscopy</b> <b>Chair Prof. Darius Abramavičius</b>
9:15-10:00	Invited lecture	<b>Leonas Valkūnas</b> ( <i>Vilnius University, Lithuania</i> ) "Roots and fruits of excitons"
10:00-10:30	Invited	<b>Michael Thorwart</b> ( <i>Universität Hamburg, Germany</i> ) "Vibronic quantum coherence at ultralow temperatures in photosynthetic protein complexes"
10:30-11:00		Coffee break
11:00-12:30		<b>Section 2: Exciton Dynamics and Spectroscopy</b> <b>Chair Prof. Donatas Zigmantas</b>
11:00-11:30	Invited	<b>Jianshu Cao</b> ( <i>Cambridge, USA</i> ) "Quantum Coherence in Excitation Energy Transfer"
11:30-11:50	Oral	<b>Rokas Jasiūnas</b> ( <i>Lithuania</i> ) "Charge Carrier Back Transfer in Non-Fullerene Organic Solar Cells"
11:50-12:10	Oral	<b>Vitalii Boiko</b> ( <i>Poland</i> ) "Trap type determination in luminescence ceramics: an approach combining Raman and Thermoluminescence spectroscopy"
12:10-12:30	Oral	<b>Karolina Maleckaitė</b> ( <i>Lithuania</i> ) "Red fluorescent BODIPY molecular rotors for lifetime-based sensing of microviscosity"

<b>12:30-13:30</b>		<b>Lunch</b>
<b>13:30-15:00</b>		<b>Section 3: Exciton Dynamics and Spectroscopy</b> <b>Chair Prof. Michael Thorwart</b>
13:30-14:00	Invited	<b>Donatas Zigmantas</b> ( <i>Lund University, Sweden</i> ) “Radiative transitions and relaxation pathways in plexcitons”
14:00-14:20	Oral	<b>Tomas Polivka</b> ( <i>Czech Republic</i> ) “On the origin of high-energy excited states of carotenoids: Multi-pulse vs. direct excitation”
14:20-14:40	Oral	<b>Joachim Seibt</b> ( <i>Austria</i> ) “Signatures of intramolecular vibrational and vibronic Qx-Qy coupling effects in absorption and CD spectra of chlorophyll dimers”
14:40-15:00	Oral	<b>Regimantas Januskevicius</b> ( <i>EKSPLA, Lithuania</i> ) „Laser light sources for spectroscopy“
<b>15:00-15:30</b>		<b>Coffee break</b>
<b>15:30-17:30</b>		<b>Section 4: Tutorial section</b> <b>Chair Assoc. Prof. Mindaugas Macernis</b>
15:30-16:00	Invited	<b>Yuri Svirko</b> ( <i>University of Eastern Finland, Finland</i> ) “Exciton-exciton interaction and resonant third-order nonlinear optical response at the semiconductor band edge”
16:00-16:30	Invited	<b>Jevgenij Chmeliov</b> ( <i>Vilnius University, Lithuania</i> ) “Exploiting the Supercomputer facilities in physical science: Identifying molecular origin of different conformational states of the pigment–protein complexes”
16:30-17:30	Workshop	<b>Laurynas Diska, Mindaugas Mačernis</b> ( <i>Lithuania</i> ) „Introduction into supercomputers and the first steps to use supercomputer ( <i>EuroCC, Lithuania</i> )“ <i>Requirements: notebook, internet access</i>
<b>17:00-17:30</b>		<b>Coffee break</b>
<b>17:30-19:00</b>		<b>Poster session: Exciton Dynamics and Spectroscopy</b>

<b>25 August</b>		
<b>9:00-10:30</b>		<b>Section 5: Exciton Dynamics and Spectroscopy</b> <b>Chair Prof. Leonas Valkūnas</b>
9:00-9:30	Invited	<b>Bruno Robert</b> ( <i>University Paris-Saclay, France</i> ) “Low frequency modes in photosynthetic pigments and proteins”
9:30-10:00	Invited	<b>Arvi Freiberg</b> ( <i>University of Tartu, Estonia</i> ) “Exciton prominence in color tuning of light-harvesting”
10:00-10:30	Invited	<b>Thomas Renger</b> ( <i>JKU Linz, Austria</i> ) “Theory of Energy Transfer in the Fenna-Matthews-Olson Trimer”
<b>10:30-11:00</b>		<b>Coffee break</b>
<b>11:00-12:30</b>		<b>Section 6: Modeling Exciton Dynamics</b> <b>Chair Prof. Yuri Svirko</b>

11:00-11:30	Invited	<b>Thomas L.C. Jansen</b> ( <i>University of Groningen, The Netherlands</i> ) "Modeling Exciton Dynamics and Spectroscopy of Natural Light-Harvesting (Super) Complexes"
11:30-11:50	Oral	<b>Florian Otterpohl</b> ( <i>Germany</i> ) "The Hidden Phase of the Spin-Boson Model"
11:50-12:10	Oral	<b>Jaemin Lim</b> ( <i>Germany</i> ) "Multimode vibronic effects in photosynthetic systems"
12:10-12:30	Oral	<b>Jakub Dostál</b> ( <i>Czech Republic</i> ) "Nonresonant Coherent Two-Dimensional Spectroscopy"
<b>12:30-13:30</b>		<b>Lunch</b>
<b>13:30-15:00</b>		<b>Section 7: Ultrafast Spectroscopy</b> <b>Chair Prof. Vidmantas Gulbinas</b>
13:30-14:00	Invited	<b>Juergen Hauer</b> ( <i>Technical University of Munich, German</i> ) "Molecular annihilation dynamics measured in the perturbative regime of excitation"
14:00-14:20	Oral	<b>Frantisek Sanda</b> ( <i>Czech Republic</i> ) "What can be learnt from 2D line-shape analysis of the fifth order signals?"
14:20-14:40	Oral	<b>Christopher Duffy</b> ( <i>England</i> ) "Exciton Migration, Annihilation and Quenching in LHCII Aggregates: Identifying the NPQ Mechanism with Fluorescence Lifetime Measurements"
14:40-15:00	Oral	<b>Light Conversion</b> "Light Conversion for Ultrafast Spectroscopy"
<b>15:00-15:30</b>		<b>Coffee break</b>
<b>15:30-17:00</b>		<b>EXCURSION to EKSPLA or Light Conversion</b>
<b>17:00</b>		<b>Departure by bus to Trakai region</b>
<b>19:00</b>		<b>CONFERENCE DINNER</b>

<b>26 August</b>		
<b>9:00-10:30</b>		<b>Section 8: Exciton Dynamics and Spectroscopy</b> <b>Chair Prof. Arvi Freiberg</b>
9:00-9:30	Invited	<b>Ulrich Kleinekathoefer</b> ( <i>Jacobs University, Germany</i> ) "Multi-scale modelling of spectral densities and absorption spectra from different light-harvesting complexes"
9:30-9:50	Oral	<b>Pavel Malý</b> ( <i>Czech Republic</i> ) "Multi-excitonic probes of coherent-to-diffusive dynamics"
9:50-10:10	Oral	<b>Saulius Bagdonas</b> ( <i>Lithuania</i> ) "Excitation energy transfer in J-aggregates of meso-tetra-(4-sulfonatophenyl) porphyrin"

10:10-10:30	Oral	<b>Arvydas Ruseckas</b> ( <i>Scotland</i> ) “Understanding the morphology of organic bulk heterojunctions using energy transfer and exciton diffusion”
<b>10:30-11:00</b>		<b>Coffee break</b>
<b>11:00-12:30</b>		<b>Section 9: Exciton Dynamics and Spectroscopy</b> <b>Chair Prof. Thomas Renger</b>
11:00-11:30	Invited	<b>Thorsten Hansen</b> ( <i>University of Copenhagen, Denmark</i> ) “Electron transfer in non-equilibrium environments”
11:30-11:50	Oral	<b>Mindaugas Macernis</b> ( <i>Lithuania</i> ) “Challenges for modeling excited states and Raman spectra properties for carotenoids and complexes with them”
11:50-12:10	Oral	<b>Erić Vesna</b> ( <i>The Netherlands</i> ) “Spectral simulations elucidate effects of structural disorder on ultrafast exciton dynamics in chlorosomes”
12:10-12:30	Oral	<b>Stepas Toliautas</b> ( <i>Lithuania</i> ) “Tracking photoexcitation to sense environment: design of BODIPY-based molecular rotors”
<b>12:30-13:00</b>		<b>Closing Remarks</b>
<b>13:00-14:00</b>		<b>Lunch</b>
<b>14:00-16:00</b>		<b>EXCURSION to Light Conversion</b>

## Poster session: Exciton Dynamics and Spectroscopy

<b>P1</b>	<b>Chris Rehhagen</b> ( <i>Germany</i> ) “Singlet and Excimer Exciton Mobility in Perylene Orange Nanoparticles”
<b>P2</b>	<b>Mykhailo Chaika</b> ( <i>Poland</i> ) “Multiphoton ionization phenomena in Cr-doped transparent garnet ceramics”
<b>P3</b>	<b>Callum Gray</b> ( <i>UK</i> ) “Energy migration and quenching models in LHCII”
<b>P4</b>	<b>Petra Čubáková</b> ( <i>Czech Republic</i> ) “Evolution of the excited state dynamics of fucoxanthin studied by Femtosecond Stimulated Raman Spectroscopy”
<b>P5</b>	<b>Martyna Patera</b> ( <i>Poland</i> ) “Crystal Phase Quantum Dots: Excitonic Calculation in Electric Fields”
<b>P6</b>	<b>Laura Baliulytė</b> ( <i>Lithuania</i> ) “Quantum-chemical study on TPPS4 monomers and dimers including their spectra”
<b>P7</b>	<b>Yaraslau Padrez</b> ( <i>Lithuania</i> ) “Dynamic spectroscopic properties of single-crystal diamond needles synthesized by different methods”
<b>P8</b>	<b>Lea Northcote Sørensen</b> ( <i>Denmark</i> ) “Charge Separation in Nature”
<b>P9</b>	<b>Long Nguyen</b> ( <i>The Netherlands</i> ) “Studying energy transfer dynamics in photosystem II complexes using 2D electronic spectroscopy”
<b>P10</b>	<b>Mantas Jakučionis</b> ( <i>Lithuania</i> ) “Modeling molecular aggregate spectra using Dirac-Frenkel variational method”
<b>P11</b>	<b>Vytautas Bubilaitis</b> ( <i>Lithuania</i> ) “Nonlinear exciton equations at fifth order to the optical field: Intensity dependent nonlinear spectra dynamics in J-type aggregate”

<b>P12</b>	<b>Gabrielė Kareivaitė</b> ( <i>Lithuania</i> ) “Changes in spectral properties of <i>trans</i> -stilbene induced by aggregates formation”
<b>P13</b>	<b>Vasyl Veremeienko</b> ( <i>France</i> ) “Singlet exciton fission mechanisms in carotenoids with strong excitonic interactions”
<b>P14</b>	<b>Lena Golubewa</b> ( <i>Lithuania</i> ) “Single-walled carbon nanotubes for photothermoacoustic destruction of cancer cells”
<b>P15</b>	<b>Kai Zhong</b> ( <i>The Netherlands</i> ) “A New Method for Excitation Transfer Applied to the LH2 System”