DIOSCURI
CENTRES OF EXCELLENCE

REGISTRATION FORM FOR CZECH SCIENTIFIC INSTITUTION

1. Research institution data (name and address):

Faculty of Mathematics and Physics
Charles University
Ovocný trh 560
116 36 Praha 1

2. Type of research institution: Public university (veřejná vysoká škola)

3. Head of the institution: Prof. MUDr. Milena Králíčková, Ph.D. – Rector

4. Contact information of designated person(s) for applicants:

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5. Research discipline in which the strong international position of the institution ensures establishing a Dioscuri Centre:

Natural Sciences and Technology: *Physical and analytical chemical sciences* - physical chemistry/chemical physics, theoretical chemistry, analytical chemistry, inorganic chemistry, organic chemistry, method development

6. Description of important research achievements from the selected discipline from the last 5 years including a list of the most important publications, patents, or other results:

The School of Physics of the Faculty of Mathematics and Physics conducts a broad spectrum of scientific research in most disciplines of physics. The research area in which the school is looking for Dioscuri Center (DC) leader candidates comprises the **experimental and theoretical chemical physics** directed towards the study of **complex chemical and biological systems** in interaction with light and their complex environments. In the theoretical line of research, the school has established itself as a home of excellent expertise in the theory of timeresolved non-linear spectroscopy, theory of photo-induced dynamics of molecular systems, including photosynthetic antennae and other biological systems exhibiting quantum effects. Recent achievements comprise identification (with experimental partners) of the so-called vibronic quasi-resonances as potential probes for dark electronic states[1], significant contributions to the development of the field of quantum biology[2], and progress in the theory of experimental techniques of coherent time resolved spectroscopy[3] including the subtleties of their interpretation[4]. *Ab initio* molecular dynamics simulations are being developed for molecular systems in the condensed phase, with a focus on aqueous solutions and other liquids, hydrogen bonding, and reactivity[5]. The strength of the theoretical environment at the School of Physics is in the ability to support experimental research in wide range of chemical physics subfields, demonstrated by excellent publications produced in collaboration with other local institutions[6,7]. On the experimental frontier, important insights into photoprotective mechanisms of photosynthetic systems[8] and photocurrent generation on artificial hybrid systems[9] have been recently obtained by a combination of time-resolved spectroscopy methods, in close collaboration with national and international groups.

- Policht, V. R. et al. Hidden vibronic and excitonic structure and vibronic coherence transfer in the bacterial reaction center. Sci. Adv. 8, eabk0953 (2022).
- Cao, J. et al. Quantum biology revisited. Sci. Adv. 6, eaaz4888 (2020).
- Malý, P. & Mančal, T. Signatures of Exciton Delocalization and Exciton - Exciton Annihilation in Fluorescence-Detected Two-Dimensional Coherent Spectroscopy. J. Phys. Chem. Lett. 9, 5654–5659 (2018).
- Kühn, O., Mančal, T. & Pullerits, T. Interpreting Fluorescence Detected Two-Dimensional Electronic Spectroscopy. J. Phys. Chem. Lett. 11, (2020).
- Brezina, K., Jungwirth, P. & Marsalek, O. Benzene Radical Anion in the Context of the Birch Reduction: When Solvation Is the Key. J. Phys. Chem. Lett. 11, 6032–6038 (2020).
- Buttersack, T. et al. Photoelectron spectra of alkali metal-ammonia microjets: From blue electrolyte to bronze metal. Science. 368, 1086–1091 (2020).
- Berger, J. et al. Quantum dissipation driven by electron transfer within a single molecule investigated with atomic force microscopy. Nat. Commun. 11, 1–10 (2020).
- Psencik, J., Hey, D., Grimm, B. & Lokstein, H. Photoprotection of photosynthetic pigments in plant onehelix protein 1/2 heterodimers. J. Phys. Chem. Lett. 9387–9392 (2020) doi:10.1021/acs.jpclett.0c02660.
- Furuya, R., Omagari, S., Tan, Q., Lokstein, H. & Vacha, M. Enhancement of the Photocurrent of a Single Photosystem i Complex by the Localized Plasmon of a Gold Nanorod. J. Am. Chem. Soc. 143, 13167– 13174 (2021).

7. List of no more than 3 important research projects in the selected discipline awarded in national and international calls to the institution in the last 5 years:

Trans-Spin NanoArchitectures: from birth to functionalities in magnetic in field

Prof. Jana Kalbáčová – Vejpravová

ERC Starting Grant

1.500.000 EUR

Accuracy and precision for molecular solids

Dr. Jiří Klimeš

ERC Starting Grant

924.375 EUR

Quantum theory of excitation energy transfer and advanced optical spectroscopy: from small dye molecules to light-harvesting complexes

Prof. Tomáš Mančal

Czech Science Foundation

EUR 370.000

8. Description of the available laboratory and office space for a Dioscuri Centre:

Time-resolved fluorescence microscopy laboratory
The spectroscopic laboratory at the Biophysics division of the Institute of Physics (IOP) of Charles University provides pulsed laser excitation tunable from 230 nm to 4000 nm continuously, detection of delay times from ~20 ps to microseconds by time-correlated single photon counting. Laboratory allows measurement of multi-channel fluorescence imaging, fluorescence lifetime imaging, resonance energy transfer, fluorescence anisotropy or twophoton fluorescence.

Two-dimensional electronic spectroscopy (2DES) laboratory

The laboratory of 2DES belongs to Department of Chemical Physics and Optics DCPO. 2DES is an advanced technique of optical spectroscopy that combines high temporal (<50 fs) and spectral resolution in range 600 nm – 800 nm. The method allows to obtain information about the kinetics of the molecular processes, such as excitation energy transfer, but also about the interactions between the molecules within the studied systems. Similar as in two-dimensional nuclear magnetic resonance, cross-peaks can be resolved in the case of coupling, which allows for direct spectral identification of the states involved in the interactions. To study slower processes occurring on a nanosecond-to-millisecond time scale, the pump-probe setup with nanosecond resolution can be used.

Raman spectroscopy laboratories

These laboratories belong to Division of Biomolecular Physics of the IOP. They feature several commercial as well as home-built Raman spectrometers and microscopes for measurement of vibrational spectra of bulk samples with high spectral resolution at several excitation wavelengths from UV to near-IR, for cell and tissue imaging as well as high-resolution nanoscale surface characterization. Raman spectrometers are accompanied by further methods such as Raman optical activity for chiral samples, or Fourier-Transform Infra-Red spectrometers for complementary vibrational spectra.

Other resources

Sample preparation and characterization laboratories feature standard equipment for biological sample handling and preparation, as well as characterization (chemical, biophysical, optical). Office-space for a team of up to 5-6 researchers dedicated to the DC is located in the center of Prague, in three floors of the Faculty of Mathematics and Physics. The center will be provided a local (i.e. physically accessible, customizable and extensible) computer cluster in an airconditioned room. A faculty operated computer cluster for high-performance computing is available to the DC researchers, with the advantage of dedicated maintenance personnel and pool of software resources.

9. List of the available research equipment for a Dioscuri Centre:

Time-resolved fluorescence microscopy

Inverted confocal fluorescence microscope (IX-83 with FV2000 scanner, Olympus), equipped with time-correlated single-photon counting (TCSPC, SPC150 electronic, Becker-Hickl) detection using hybrid photo-multipliers (Hamamatsu) or APDs. FLIM (PicoQuant) and 16- channel spectral FLIM (Becker-Hickl). Time range of detection from ~20 ps to μs. Excitation is provided by a tunable pulsed laser (Chameleon Ultra II, Coherent) with Compact-OPO (Coherent) with optional doubling or tripling, wavelength range 230 nm to 4000 nm continuous, pulses 150 fs, 80 MHz with optional pulse picker (APE). Alternative excitation by pulsed diodes (PicoQuant). For bulk measurements fiber-based spectrofluorometer (TIDAS, J&M) is available.

Two-dimensional electronic spectroscopy (2DES) and transient absorption (TA)

The available setup for 2DES and TA uses amplified femtosecond pulses from a regenerative amplifier (Pharos-6W, Light Conversion), 200 kHz repetition rate. Two non-collinear optical parametric amplifiers (Orpheus-N-3H and Orpheus-N-2H, Light Conversion, ~300-1000 nm) can be pumped simultaneously producing ~30 fs pulses, 100 nm bandwidth, range 600 – 800 nm. The signal passes through an imaging spectrometer (IsoPlane 160, Princeton Instruments) and is detected on electron multiplying CCD camera (PRoEM+ 16002 eXelon3, Princeton Instruments). A setup for long-delay TA (ns to ms) uses for excitation ~3 ns (FWHM) pulses from an optical parametric oscillator (PG122, EKSPLA, ~210-355 & 420-2300 nm) pumped by a Q-switched Nd:YAG laser (NL303G/TH, EKSPLA) and a Xenon flash lamp (Perkin Elmer) for probe pulses. Detection by intensified CCD camera (PI-MAX 512RB, Roper Scientific, 200-850 nm) coupled to an imaging spectrometer (iHR 320, Horiba Jobin Yvon).

Raman spectroscopy

Versatile confocal Raman microscope WITec alpha300 RSA combined with atomic force (AFM) and scanning near-field optical microscope (SNOM). The WITec system is equipped with 442, 532, 633, 647, 785, 830 nm excitations, two multi-grating spectrographs with optimized CCD detectors allowing efficient detection of Raman as well as fluorescence signal, and polarization modules. Furthermore, confocal Raman microscope LabRam HR800 (Horiba Jobin-Yvon) equipped with excitations 488, 514, 633, 785 nm, a modular macro-Raman spectrometer with 442, 488, 514, 532 nm excitations, and an in-house-built UV Raman spectrometer with 229, 244, 248 and 256 nm excitations are available. Further spectroscopic methods, e.g., Raman optical activity (home-built), UV-Vis absorption (Perkin-Elmer, Analytik Jena), FTIR (Bruker), vibrational and electronic circular dichroism (BioTools), dynamic light scattering can be used as well.

Sample preparation and characterization

Standard equipment for biological sample handling and preparation (wet labs), such as flowbox, fume hoods, shakers, incubators, electrophoresis, sonicator, centrifuge (Hettich), vacuum concentrator (Eppendorf/Scanvac), analytical balances, pH meters, autoclave, dry ice machine, deionized water

(UHQII, Elstat) etc. Optical characterization includes steady-state UV-VIS absorption spectrometers (Varian Cary, Perkin-Elmer, Specord), fluorescence spectrometers (Fluoromax 2,3,4, Horiba). Tabletop microscopes (TM-1000, Hitachi, IX70, Olympus, Zeiss) are available as well.

Computational resources

Numerical simulations and related computational tasks can be performed with a hierarchy of hardware and software means available to the researchers of the DC. The center will be provided a local (i.e. physically accessible, customizable and extensible) computer cluster in an airconditioned room, equipped with multi-core Linux workstations with 8 to 32 cores (Intel Xeon) and up to 64 GB of memory each and several GPUs. A faculty operated computer cluster for high-performance computing is available to the DC researchers, with the advantage of dedicated maintenance personnel and pool of software resources. On the highest level of this hierarchy is the national distributed computing infrastructure (Metacentrum), membership of which is available to researchers for all academic institutions with the Czech Republic. Metacentrum provides software and hardware support for large scale, memory and CPU intensive computations, and high-performance GPU workstations.

10. List of the additional benefits (other than listed in the conditions for hosting a DC, see invitation) that the Institution declares to provide for a Dioscuri Centre (i.e.: additional funds, personal benefits, dual career options, relocation support or other):

The School of Physics offers all employees additional benefits according to the rules of the School, and all benefits that the University provides as a whole; Charles University is the European HR Award (Human Resources Award) holder. Part-time and temporary contracts are common and easily amended according to the needs of employees. Among the benefits, supplemental pension fund contribution is offered to permanent staff, as are meal subsidies, personal development days and sick days, and all the benefits according to Labour Law (min. 5 weeks of vacation (8 for teaching/academic staff), full social security and healthcare insurance, etc.). International relocation staff at the school will help with securing visa (if necessary), initial health insurance, information on suitable accommodation, personal mobile phone and data services, establishing bank account, etc. Depending of the country of origin, relocation support can be offered.

11. Other information about the internationalization of the research institution, international researchers employed at the institution, the availability of English language seminars etc.:

The School of Physics of the Faculty of Mathematics and Physics provides a highly internationally connected research environment. All faculty members have a long-term international research experience and keep scientific collaborations with top international institutions in Europe and world-wide. This creates a vibrant international setting open to and quickly reacting to global scientific development. In the field, in which the DC is projected to conduct its research, the faculty has one truly international senior member (out of five), most other senior researchers have roots in the Czech Republic with scientific ties to international institutions. There is a steady turnaround of international postdocs with about 20 – 30 accepted every year. The School accepts about 100 PhD students into its graduate program each year, with the ratio of more than 50 % of international PhD students among the newly accepted. Local seminars are conducted in English as a rule whenever international faculty members, students or researchers are present. For future students at PhD level associated with the DC, lectures in English in topics related to the relevant field(s) of research are available, e.g., as a part of the EU4+ European University Alliance.