



# ABSTRACTS

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# Spatio-temporal characterization of few-cycle 3.2 $\mu\text{m}$ pulses from a mid-IR OPCPA system

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Four-cycle pulses from a 3.2  $\mu\text{m}$  OPCPA system were characterized by spatially resolved Fourier transform spectroscopy, for the first time. Combining the spatio-spectral information with temporal characterization yielded the spatio-temporal structure of the pulses revealing up to now inaccessible details in the mid-IR spectral region. The proposed technique offers efficient and simple characterization for the optimization of MIR OPCPA systems in terms of spatio-spectral couplings.

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# Impact of material properties on the nonlinear spectral broadening in thin solid media

● V. Pajer, L. Lehotai, J. Bohus, B. Tari, M. Kalashnikov, Á. Börzsönyi, and R. S. Nagymihály

We present the post-compression of 25 fs pulses with a flat-top beam profile in different nonlinear media. Fused silica, sapphire, and YAG plates were tested for spectral broadening and compressibility while measuring the spatio-spectral properties of the broadened pulses. To our best knowledge, such systematic investigation has not yet been carried out. The near- and far-field profiles show that no significant wavefront distortion occurred during the nonlinear propagation but the spatio-spectral homogeneity has a strong correlation with the material characteristics and the accumulated B integral. A series of numerical simulations were also conducted to have deeper insight on the broadening process and the impact of the material properties. The theoretical model also reveals the limitations of compressibility in the single thin plate arrangement and it can support the optimization of future, high-energy experiments.

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**Optics Communications**  
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# Rapid-scan pulse-shaper-assisted two-dimensional electronic spectroscopy of Photosystem I using high-repetition-rate supercontinuum pulses

● S. Singhal, P. Akhtaar, F. Sarlós, G. Sipka, Á. Sipos, P. Jójárt, B. Gilicze, I. Seres, Zs. Bengery, T. N. Do, H-S. Tan, and P. H. Lambrev

An ultrafast optical spectrometer is constructed, relying on a Yb fiber-based fewcycle laser system to generate high-repetition-rate (100 kHz) pulses and employing white-light supercontinuum in a pump-probe beam configuration for transient absorption spectroscopy (TAS) and two-dimensional electronic spectroscopy (2DES). The instrument benefits from shot-to-shot pulse shaping and detection for a reduced background noise, improving the sensitivity of the method and the ability to record TAS and 2DES with low pulse energies and short acquisition time, which can be critical for measuring the dynamics of biological systems. The practical applicability of the instrument is demonstrated by performing TAS and 2DES on trimeric Photosystem I complexes, isolated from the cyanobacterium *T. vulcanus*. It is also shown that rich, biophysically relevant information can be extracted from the combination of short TAS and 2DES measurements. The approach is employed to ascertain the main timescales of transfer and trapping of excitations among different Chl pools in the *T. vulcanus* PSI.

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# PI-FROSt characterization of solid-state harmonics with spectra spanning over 2.6 octaves

● P. Béjot, B. Kiss, R. Shrestha, L. Ábrók, Z. Kis, K. Pirisi, B. Bagó, O. Faucher, F. Billard, E. Cormier and E. Hertz

We present a comprehensive characterization of an ultra-broadband laser field across the visible–mid-infrared (MIR) spectral region. The radiation consists of a series of harmonic fields generated in a ZnO crystal by a long-wavelength, few-cycle driving pulse operating at 100 kHz. The characterization relies on the recently developed Plasma-Induced Frequency Resolved Optical Switching (PI-FROSt) method. In this study, we demonstrate the ability of this straightforward method to characterize, with the same nonlinear architecture, the MIR driving field centered at a wavelength around 3.2  $\mu\text{m}$ , along with all (odd and even) harmonics up to the fifth order. The total spectrum spans over an exceptionally broad bandwidth of 2.6 octaves, ranging from 0.59 to 3.6  $\mu\text{m}$ . All assessments confirm the high reliability and suitability of PI-FROSt for the metrology of over-octave-spanning waveforms, representing an effective solution for characterizing unconventional secondary sources. The field reconstruction provides valuable insights into the generation mechanisms, which can serve as a guideline to support numerical modeling.

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# Continuous high-yield fast neutron generation with few-cycle laser pulses at 10 Hz for applications

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We present a laser-based neutron source that produces  $1.8 \times 10^5$  neutrons/s with a conversion rate of  $7.8 \times 10^5$  neutrons/J. Laser pulses of 12 fs and 23 mJ were focused onto a 430-nm-thick heavy water liquid sheet at a 10 Hz repetition rate. The resulting peak intensity of  $4 \times 10^{18}$  W/cm<sup>2</sup> accelerated deuterium ions from the target rear side to a kinetic energy of 1 MeV. This deuteron beam induced  ${}^2\text{H}(d, n){}^3\text{He}$  fusion reactions in a deuterated polyethylene target, producing fast neutrons. The neutron yield was measured using two independent detection systems: the LILITH time-of-flight spectrometer, consisting of eight plastic scintillators covering nearly 180°, and a calibrated bubble detector spectrometer. The neutron yield per laser shot is 35 times higher than that recently achieved by lasers with comparable pulse energies, while the conversion rate is the highest ever achieved by continuously operating, sub-100 fs lasers. The generated neutrons are emitted from an area of 0.65 cm<sup>2</sup> corresponding to the deuteron beam spot on the catcher. Their angular distribution is peaked in forward and backward directions in agreement with the literature data on the angular distribution of  ${}^2\text{H}(d, n){}^3\text{He}$  reaction. The system operated continuously for several hours per day with an unprecedented stability of 5%.

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# Distinguished role of the laser pulse temporal structure on deuteron acceleration

● P. Varmazyar, Zs. Lécz, Sz. Tóth, T. Gilinger, B. Nagy, J. Csontos, M. Füle, and K. Osvay

Compared to their conventional counterpart, laser plasma-based ion accelerators offer considerably higher acceleration gradients, opening the way to more compact laser-driven accelerator facilities. In this context, deuteron acceleration has been used for laser-based neutron sources, as deuterons at relatively low kinetic energy can efficiently generate neutrons. While double-pulse and chirp effects have been explored for proton acceleration under radiation pressure and target-normal sheath acceleration schemes, their role in ion acceleration remains unconfirmed, limiting the optimization strategies for neutron sources. Here we clarify the influence of laser pulse temporal shape on ion acceleration from ultrathin targets. We systematically change the temporal structure of the pulse by controlling the group delay dispersion and third-order dispersion (TOD), while pulse energy and focal spot size remain unchanged. The experiments are supported by 2D PIC simulations and analytical modeling. We find that the effect of optimum temporal shape is considerably larger than previously reported: the TOD-induced post-pulses increase the efficiency by 50% and double the deuteron cutoff energy. Our systematic study shows that the performance of laser ion accelerators can be strongly enhanced by matching the dispersion values to the target characteristics.

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# Dynamic interference of chirped photoelectrons

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Dynamic interference is an elusive strong-field effect where photoelectrons from intense laser pulses interfere in time, forming rich kinetic energy patterns. Here, we present the first experimental demonstration of isolated dynamic interference using a novel two-color scheme: chirped laser-assisted dynamic interference. Isolation was achieved with a crossed-polarization setup combining an extreme ultraviolet harmonic field and an infrared pulse with tailored spectrotemporal properties. Beyond prior works, our approach enables precise control over interfering trajectories, yielding holographic interference patterns and advancing our understanding of strong-field phenomena.

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# Active stabilization for ultralong acquisitions in an attosecond pump-probe beamline

● T. Csizmadia, L. Gulyás Oldal, B. Gilicze, D. S. Kiss, T. Bartyik, K. Varjú, S. Kahaly, and B. Major

Attosecond time-resolution experiments using noncollinear interferometers require precise and active control of the optical delay to prevent instabilities—including both slow drifts and rapid vibrations—that can obscure the time evolution of the physical system under investigation. In this work, we present the design and results of stability measurements for a double interferometer setup, consisting of a two-color interferometer for extreme ultraviolet-infrared pump-probe spectroscopy complemented by a single color auxiliary interferometer designed for active delay stabilization. The attosecond pump-probe setup is driven by a high-average-power, high-repetition-rate laser system and offers sub-optical-cycle ( $\pm 81$  as) stability with a fast feedback rate over extended periods (up to several days). Due to the noncollinear arrangement, the setup enables independent control of both amplitude and phase, such as controlling the XUV spectrum or attochirp, or the IR dispersion and carrier-envelope phase in the two arms, even across significantly different spectral regions. As a proof of concept, we demonstrate attosecond beating in angle-resolved photoemission during two-photon, two-color photoionization, highlighting the broad potential of the system for kinematically and dynamically complete studies of atomic-scale light-matter interactions.

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# Attosecond temporal structure of non-consecutive harmonic combs revealed by multiple near-infrared photon transitions in two-color photoionisation

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The metrology of attosecond pulse trains is based on a cross-correlation technique between a comb of extreme ultraviolet harmonics generated by the high-order harmonic generation process and a synchronised infrared field. The approach, usually referred to as reconstruction of attosecond beating by interference of two-photon transitions (RABBIT), allows one to recover the relative phase between the comb of consecutive odd harmonics, thus providing access to the attosecond temporal structure of the radiation. Seeded free-electron lasers have recently demonstrated the generation of combs consisting of even and odd harmonics of the seeding radiation. In this scheme, each harmonic is generated by an independent undulator (or set thereof), providing an additional degree of freedom in selecting the specific harmonics that make up the extreme ultraviolet comb. Here, we present results on the generation and temporal characterisation of a comb consisting of non-consecutive harmonics. The single-shot correlation analysis of the photoelectron spectra and the reordering of the single-shot data using an attosecond timing tool allow the reconstruction of the group delay dispersion of the harmonic comb and the temporal reconstruction of the attosecond pulse train.

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**Communications Physics**  
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# Nonlinear optics using intense optical coherent state superpositions

● Th. Lamprou, J. Rivera-Dean, P. Stammer, M. Lewenstein, and P. Tzallas

Superpositions of coherent light states are vital for quantum technologies. However, restrictions in existing state preparation and characterization schemes, in combination with decoherence effects, prevent their intensity enhancement and implementation in nonlinear optics. Here, by developing a decoherence-free approach, we generate intense femtosecond-duration infrared coherent state superpositions (CSSs) with a mean photon number orders of magnitude higher than the existing CSS sources. We utilize them in nonlinear optics to drive the second harmonic generation process in an optical crystal. We experimentally and theoretically show that the nonclassical nature of the intense infrared CSS is imprinted in the second-order autocorrelation traces. Additionally, theoretical analysis shows that the quantum features of the infrared CSS are also present in the generated second harmonic. The findings introduce the optical CSS into the realm of nonlinear quantum optics, opening up new paths in quantum information science and quantum light engineering by creating nonclassical light states in various spectral regions via nonlinear up-conversion processes.

SeSo

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# Attosecond metrology of vacuum-ultraviolet high-order harmonics generated in semiconductors via laser-dressed photoionization of alkali metals

● A. Nayak, D. Rajak, B. Farkas, C. Granados, Ph. Stammer, J. Rivera-Dean, Th. Lamprou, K. Varjú, Y. Mairesse, M. F. Ciappina, M. Lewenstein, and P. Tzallas

Semiconductor crystals driven by strong mid-infrared pulses offer advantages for studying many-body physics and ultrafast optoelectronics via high-harmonic generation. While the process has been used to study solids in the presence strong mid-infrared fields, its potential as an attosecond light source is largely underexplored. We demonstrate that high-harmonics emitted from zinc-oxide crystals produce attosecond pulses, measured through spectroscopy of alkali metals. Using a cross-correlation approach, we photoionize Cesium atoms with vacuum-ultraviolet high-harmonics in the presence of a mid-infrared laser field. We observe oscillations in the photoelectron yield, originating from the instantaneous polarization of atoms by the laser field. The phase of these oscillations encodes the attosecond synchronization of the high-harmonics and is used for attosecond pulse metrology. This source opens new spectral windows for attosecond spectroscopy, enabling studies of bound-state dynamics in natural systems with low ionization energies, while facilitating the generation of non-classical entangled light states in the visible-VUV.

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# Recent developments in the generation of non-classical and entangled light states using intense laser-matter interactions

● Th. Lamprou, P. Stammer, J. Rivera-Dean, N. Tsatrafyllis, M. F. Ciappina, M. Lewenstein, and P. Tzallas

Non-classical and entangled light states are of fundamental interest in quantum mechanics and they are a powerful tool for the emergence of new quantum technologies. The development of methods that can lead to the generation of such light states is therefore of high importance. Recently, it has been demonstrated that intense laser-matter interactions can serve towards this direction. Specifically, it has been shown how the use of fully quantized approaches in intense laser-matter interactions and the process of high harmonic generation, can lead to the generation of high photon-number non-classical and entangled states from the far-infrared to the extreme-ultraviolet. Here, after a brief introduction on the fundamentals, we summarize the operation principles of these approaches and discuss the recent developments and future directions of non-classical light engineering using strong light fields with the potential application in ultrafast and quantum information science. These findings represent an important step in the development of novel quantum nonlinear spectroscopy methods, based on the interplay between the quantum properties of light and those of quantum matter.

SeSo

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# Investigation of pre-pulse effects on ultrashort-pulse laser interaction with structured targets

● A. Kim, I. Dey, A. Bepaly, P. Komm, A. Shaham, J. Papeer, M. Botton, and A. Zigler

The role of pre-plasma in the efficient generation of protons by intense laser-matter interaction from structured targets is investigated. Optimal energy coupling between laser and plasma is found by varying the fluence and arrival time of an independently controllable ultrashort pre-pulse with respect to the main interaction pulse. The coupling is evaluated based on the energy of the accelerated protons. The accelerated proton energy is maximized at optimal pre-pulse delay and fluence conditions. Plasma emission spectrum and Particle-in-Cell simulations provide a possible explanation of the obtained experiment results.

SeSo

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# Stable high-energy proton acceleration with water-leaf targets driven by intense laser pulses

● L. R. He, M. Bachhammer, F. Balling, S. Biswas, L. Doyle, S. Gerlach, I. Hofrichter, M. Kharbedia, J. Liese, M. De Marco, T. Pohle, A. Praßelsperger, A.-K. Schmidt, F. Schweiger, M. F. Kling, S. Karsch, and J. Schreiber

Laser plasma acceleration techniques hold promise for generating compact, high-flux relativistic proton bunches. However, the inherent instability of laser-plasma interactions and the requirement for reliable proton source stability often hinder their practical applications. In this paper, we explore the potential of a water-leaf target irradiated by 27 fs laser pulses with energies ranging from 1.1 to 9.9 J and peak intensities spanning from  $10^{20}$  to  $10^{21}$  W/cm<sup>2</sup>. We finally conducted a series of 400 shots with a peak power of 300 TW, producing proton energies up to 30 MeV and peak flux beyond  $10^9$  protons MeV<sup>-1</sup>msr<sup>-1</sup>. These results demonstrate the possibility of long-term, stable, and efficient proton acceleration at high repetition rates, addressing a key challenge in laser-plasma acceleration.

SeSo

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# Multi-GeV electron beam generation via two-stage laser wakefield acceleration

● R. Ul Haq, M. Rezaei-Pandari, X. Xie, X. Liang, M. Sun, P. Zhu, Z. Lu, Guoli Zhang, L. Li, H. Xue, N. A. M. Hafz, and J. Zhu

Despite considerable progress in multi-stage laser wakefield acceleration (MSLWFA), efficient coupling between stages and the impact of laser–beam injection delay remains open challenges. A two-stage LWFA scheme is demonstrated using particle-in-cell (PIC) simulations, capable of producing multi-GeV electron beams over millimeter-scale propagation lengths. In the first stage, a high-intensity laser pulse (with  $a_0=7.7$ ,  $w_0=20\text{ }\mu\text{m}$ ,  $\tau=30\text{ fs}$ ,  $E=30\text{ J}$ ,  $\lambda_0=800\text{ nm}$  and  $I_0=1.2\times 10^{20}\text{ W/cm}^2$ ) propagates through a neutral helium (He) gas target inside a gas cell, with ionization modeled self-consistently to produce a fully ionized plasma at a plateau density  $7\times 10^{18}\text{ cm}^{-3}$ , generating a high-quality 1 GeV electron beam. This beam is then injected into a second stage inside the same gas cell, where systematically varying the injection delay enhances the injected bunch energy to 2.5 GeV and boosts background trapped electrons to 3 GeV, while reducing energy spread and preserving charge. These findings underscore the critical role of synchronization and plasma tailoring strategies relevant for future multi-pulse and flying-focus LWFA configurations.

SeSo

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# Ultra-high-brightness and tuneable attosecond-long electron beams with the laser wake field acceleration

● P. Tomassini, F. Avella, N. A. M. Hafz, L. Labate, V. Horný, Sz. Tóth, D. Doria, and L. A. Gizzi

Ultra-low emittance and length-tuneable electron beams can be obtained with the Laser Wake Field Acceleration (LWFA) by employing advanced ionization injection techniques, such as the Two-Color and the Resonant Multi-Pulse Ionization injection (ReMPI) schemes. There, a tightly focused, short wavelength (ionization) pulse extracts electrons from a selected inner shell of a dopant, allowing them to be longitudinally compressed and trapped in the wakefield excited by a different (driver) pulse. In this work we demonstrate, by means of analytical results and Particle In Cell simulations, that 340 as long electron beams with 2.3 GeV energy, 6.1 pC charge, 0.15% projected energy spread, 60 nm normalised emittance, and projected 6D-Brightness in excess of  $3 \times 10^{18}$  A/m<sup>2</sup>/0.1% BW can be generated with a 200 TW Ti:Sa laser system. The beam slice analysis reveals its potentialities for driving a few-spikes attosecond X-ray Free Electron Laser. Furthermore, the ultra-high projected quality, and the extreme shortness of the beams make them ideal candidates for the generation of attosecond and quasi-monochromatic  $\gamma$  photons beams through Thomson/Compton backscattering, or for the injection in subsequent plasma wakefield structures so as to reach TeV energies from staged LWFA.

SeSo

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# Single-mode laser guiding in non-parabolic plasma channels for high-energy electron acceleration

● P. Tomassini, F. Avella, N. A. M. Hafz, L. Labate, V. Horný, Sz. Tóth, D. Doria, and L. A. Gizzi

The discovery of laser wakefield acceleration in gaseous plasma was a major milestone that could lead to a significant reduction of size and cost of large electron accelerators. For higher-energy laser-driven electron acceleration guiding plasma channels were proposed, which are matched to the laser pulse parameters. For guiding a Gaussian beam, a parabolic density profile is needed, which is difficult to realize experimentally. The realistic channel profiles can be described by higher order polynomial functions which are not optimal for guiding due to the development of undesired distortions in the laser intensity envelope. However, here we show that for non-parabolic plasma channels well-defined matching conditions exist, which we call mode matching. This leads to the guiding of the fundamental mode only in the acceleration regime, where the plasma electron density is modulated by the high-intensity laser pulse. In this way we eliminate two deteriorating factors of laser wakefield acceleration, namely the mode dispersion and energy leakage. We apply this new matching condition for single-mode guiding in quasi-3D simulations to show that 10 GeV energies can be reached in a distance of less than 15 cm.

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# Enhanced THz emission from photoconductive antennas by integrating photonic structures on a semi-insulating GaAs substrate

● G. Rana, A. Gupta, A. Bhattacharya, S. P. Duttagupta, and S. S. Prabhu

Terahertz photoconductive antennas (THz PCAs) have significantly advanced the THz research by offering room-temperature operation, broad bandwidth and relatively low cost as both emitters and detectors. However, the primary limitation has been their low power output due to inefficient conversion. This article demonstrates a substantial improvement in efficiency (~200%) by incorporating sub-micron photonic structures on the surface. These photonic structures enhance pump beam coupling, leading to increased photocarrier generation. They also facilitate efficient carrier recombination after THz emission, thereby suppressing carrier screening. Experimental and numerical studies confirm the enhanced photocarrier generation and controlled transport through defect-free paths, further reducing screening effects. The integration of photonic structures into large area emitters (LAEs) holds the potential to develop emitters and detectors suitable for real-world THz systems, overcoming the limitations of the current commercial LAEs that rely on plasmonic structures or antireflection coatings. This innovation has the potential to revolutionise THz technology, enabling the development of more powerful and efficient THz sources and detectors. This can lead to advancements in various fields, including wireless communication, imaging and sensing and spectroscopy.

SeSo

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# Terahertz self-induced dynamic slow-light behavior in metasurfaces

● S. Mallick, N. Acharyya, V. Gupta, Sh. Rane, K. M. Devi, A. Sharma, J. A. Fülöp, and D. R. Chowdhury

Dynamically reconfigurable metasurfaces are complex to realize because they require exotic materials, external stimuli, or both. However, with the advent of intense THz transients, these conventional preconditions can be bypassed. Strong THz fields are capable of invoking modulation of the electronic configuration in materials through impact ionization. In this context, we report the diligent intertwining of strong THz field-induced nonlinearities and the structural interactions of near-field coupled metastructures. We experimentally demonstrate a well-established metal-on-silicon metasurface framework to achieve reconfigurability that is devoid of any exotic materials or external stimuli. Aided by meta-geometry, intense THz transients modify the dispersion of the silicon substrate, leading to self-induced nonlinear modulations in conductivities. Altering the conductivity through impact ionization results in dynamically reconfigurable electromagnetically induced transparency (EIT) effects in a self-sustained manner, controlling the slow-light characteristics (group delay and the group velocity) by more than 6 times. These outcomes could potentially enable versatile applications in upcoming 6G technologies and on-chip silicon-based integrated photonics.

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# Two-photon absorption and its saturation in organic terahertz-generator crystals NMBA, BNA, and MNA

● A. Gupta, T. Zhang, V. Hanyecz, J. Bohus, V. Gupta, A. Sharma, and J. A. Fülöp

Absorption at the pump wavelength sensitively influences the achievable terahertz (THz) generation efficiency and the damage threshold of organic THz generator crystals. In the frequently used THz-generator crystals NMBA, BNA, and MNA, we measured the intensity-dependent transmittances and determined the effective low-intensity two-photon absorption coefficients for pulses at 780 nm central wavelength. We observed the saturation of two-photon absorption in BNA and MNA and gave values for the corresponding effective saturation intensities. Our results enable better numerical models of THz generation and optical heating, with nonlinear pump absorption included, to aid the design of simple and robust strong-field THz sources using organic crystals directly pumped by femtosecond lasers.

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# Waveform-controlled field synthesis of sub-two-cycle pulses at the 100 TW peak power level

● L. Veisz, P. Fischer, S. Vardast, F. Schnur, A. Muschet, A. De Andres, S. Kaniyeri, H. Li, R. Salh, K. Ferencz, G. N. Nagy, and S. Kahaly

Ultrahigh peak-power laser systems with pulse durations of tens of femtoseconds are widely used as drivers for compact sources of particles and secondary radiation. Conversely, lasers with shorter (a few femtoseconds) pulse durations and lower peak powers enable the generation of isolated attosecond light pulses to study nature with unparalleled temporal resolution. Here we report an enhanced optical parametric chirped pulse amplifier system that produces light pulses with a peak power of about 100 TW and a pulse duration as short as 4.3 fs with full waveform control. Coherent field synthesis generates a broadband spectrum, spanning from the visible to the near infrared, through three cascaded amplification stages, each housing two optical parametric amplifiers that sequentially boost complementary spectral regions. The resulting light transients are waveform-stabilized to <300 mrad and focused to an intensity of  $10^{21} \text{ W cm}^{-2}$  and exhibit an outstanding high dynamic range in temporal contrast. Together, these characteristics render the system well suited for demanding relativistic laser–plasma experiments. Utilizing temporal super-resolution, the pulses are shortened to sub-4-fs duration. This platform is dedicated to advancing the frontiers of attosecond electron and X-ray sources.

SeSo, UFS

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# From ultrafast laser-generated radiation to clinical impact: a roadmap for radiobiology and cancer research at the Extreme Light Infrastructure (ELI)

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The extreme light infrastructure (ELI) is emerging as a state-of-the-art facility providing international users with open access to ultrashort laser-driven particle bunches, ranging from a few femtoseconds to a few nanoseconds, for advanced radiobiology studies. ELI offers femtosecond-class laser pulses and ultrafast ionizing radiation characterized by extremely high instantaneous dose rates (107–1012 Gy/s). The versatility of ELI's cutting-edge technologies enables the generation of high repetition rate (1 Hz–1 kHz) secondary sources (protons, ions, electrons, and neutrons) with energies from a few MeV to several hundred MeV, achieved over sub-millimetre to millimetre-scale acceleration lengths, along with fundamental research in the field of ultrahigh intensity laser-matter interaction based on the use of the highest peak power laser pulses available worldwide. Harnessing these laser-driven particle sources for radiobiology and medical research demands a coordinated international effort, with a strong focus on advancing scientific instrumentation and refining experimental methodologies to support progress in ultrafast laser-driven radiation biology. This roadmap underscores the need for systematically designed experiments across ELI facilities, supported by preparatory research at users' home laboratories, alongside the ongoing development of instrumentation and infrastructure. These efforts are critical to rigorously assess and validate the therapeutic potential of these novel sources, paving the way for a transformative shift in radiation biology and medicine.

## SeSo, UFS

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# Riccati equation perspective on Landau-Zener transitions

● E.. P. Glasbrenner, Y. Gerdes, S. Varró, and W. P. Schleich

We express the dynamics of the two probability amplitudes in the elementary Landau-Zener problem in terms of the solution of the corresponding Riccati differential equation and identify three key features: (i) The solution of the Riccati equation provides the bridge between the two probability amplitudes. (ii) Neglecting the nonlinearity in the Riccati equation is equivalent to the Markov approximation which yields the exact asymptotic expression for one of the probability amplitudes. (iii) The Riccati equation identifies the origin of the failure of the Markov approximation not being able to provide us, in general, with the correct asymptotic expression of the other probability amplitude. Our approach relies on approximate yet analytical solutions of the Riccati equation in different time regimes, highlighting the impact of its nonlinear nature on the time evolution of the system.

UFS

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Phys. Rev. Research  
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# Modulating band offset through interface engineering of Cu<sub>2</sub>SnSe<sub>3</sub>-based heterojunctions for efficient charge separation and collection

● D. R. Borkar, A. Mandal, Y. A. Jadhav, H. I. Eya, S. Kolekar, M. Upadhyay Kahaly, G. F. Samu, G. M. Gouda, and S. R. Rondiya

Cu<sub>2</sub>SnSe<sub>3</sub> (CTSe) shows promise due to its wide solar absorption and tunable band gap, though low efficiency caused by interface recombination and crystallinity issues remains a challenge. In this study, a systematic and facile synthesis method for CTSe nanoparticles (NPs) is demonstrated, accompanied by an in-depth analysis of their growth mechanisms. A comprehensive experimental and theoretical investigation is conducted to explore the structural, compositional, optoelectronic, and band alignment properties of p-type CTSe NPs as a solar absorber, along with n-type CdSe and ZnSe NPs as buffer layers. Additionally, the band edge positions of the synthesized NPs are estimated using cyclic voltammetry (CV), UV photoelectron spectroscopy (UPS), and density functional theory (DFT), enabling the modulation of band offsets through interface engineering. The investigation revealed a staggered type-II band alignment at the CTSe/CdSe heterojunction, characterized by a minimal conduction band offset (CBO) of 0.06 eV. The findings from CV and UPS measurement supported by density functional theory-based calculations, suggests effective charge carrier separation and transport at the interface. The CTSe/CdSe heterojunction exhibited Schottky I–V characteristics, demonstrating a current of 1 mA in dark conditions. These findings demonstrate CTSe NPs' potential as an efficient absorber in thin-film solar cells, addressing interface recombination losses and improving performance.

UFS

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Small Methods





# Development of a novel PDMS/PEG/PDMS multilayered composite film for advanced thermal management solutions for Photovoltaics

● R. S. Calolsa, T. P. Sumangala, S. K. Kalpathy, T. Thomas, M. Upadhyay Kahaly, and A. Rahaman

This study presents a novel multilayered composite thin film of polyethylene glycol (PEG4000) sandwiched between two layers of polydimethylsiloxane (PDMS) with a prime focus on improving photovoltaic device efficiency and longevity. The PDMS/PEG/PDMS configuration absorbs heat from the device and near-infrared (NIR) sunlight thereby reducing thermal buildup and preventing material degradation. PDMS/PEG/PDMS film composite was fabricated using the doctor blade technique, this hydrophobic composite undergoes a solid-to-liquid phase transition at approximately 50–60 °C, enhancing thermal energy management. In its liquid state, the film composite exhibits 85.01 % visible transmittance and 11.11 % NIR reflectance, while in solid state, it shows 62.94 % visible transmittance and 13.40 % NIR reflectance. The phase change material (PCM) maintains cyclic stability without leakage and demonstrates a transparency shift with heat absorption, indicating effective thermal cycle stability.

UFS

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# Correlation-driven ultrafast charge migration in pyrrole derivatives: the influence of the alkyl group

● G. N. Nagy, K. Chordiya, V. Despré, A. I. Kuleff, and M. Upadhyay Kahaly

Pyrrole and its derivatives are essential components of many important organic molecules. By studying their response to ionization, we can gain insights into the photo-assisted reactions they participate in, as well as understand their overall photoresponse. In this study, we examine the effect of alkyl substitution in pyrrole derivatives on the ultrafast charge-migration dynamics initiated by inner-valence ionization. Using a multielectron wave-packet propagation approach, we investigate the correlation-driven charge redistribution in pyrrole (P), N-methylpyrrole (MP), and N-ethylpyrrole (EP). Additionally, we explore the stability of the  $\pi$ -conjugation structure involving the participation of the nitrogen's lone electron pair. Our findings reveal that as the length of the alkyl chain increases, significant charge migration and charge separation dynamics occur between the pyrrole and the alkyl group with only a small increase in the timescale.

UFS

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**Phys. Chem. Chem. Phys.**  
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# PDMS/Au/PDMS Multi-Layered Thin Film Composites for Hydrophobic and IR Filtering Applications

● R. S. Calolsa, T. P. Sumangala, S. K. Kalpathy, T. Thomas, M. Upadhyay Kahaly, and A. Rahaman

This study introduces a novel PDMS/Au/PDMS multi-layered thin-film composite designed for infrared (IR) filtering and hydrophobic coating applications, fabricated using spin coating and sputtering techniques. The composite, with an approximate thickness of 30  $\mu\text{m}$ , exhibits a surface roughness that enhances near-infrared (NIR) reflectance through diffuse scattering, achieving a reflectance of up to ~60%, while maintaining visible light transmission of approximately 70%. The choice of gold as the intermediate layer in this study is motivated by its optical property of surface plasmon resonance, which significantly contributes to the material's reflective characteristics in the NIR spectrum. This unique combination of NIR reflectivity and visible light transparency makes the film ideal for applications like solar cell encapsulation, with the potential to boost photon absorption while reducing heat buildup. Additionally, this composite film shows promise as a coating for greenhouse windows and for thermal management in electronic devices, representing a significant advancement in multifunctional, energy-efficient materials.

UFS

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# Defect and solvent engineering of optoelectronic response in 2D materials: A DFT study on graphene, silicon carbide, and boron nitride for solar cell sensitizers

● M. A. Al-Seady, L. A. O. Al-Jamal, E. Ahmed, and M. Upadhyay Kahaly

In the present investigation, the geometrical, electronic, photovoltaic parameters, and optical properties of graphene (G), silicon carbide (SiC), and boron nitride (BN) nanostructures were studied using density functional theory (DFT) and time-dependent DFT (TD-DFT) methods. Dimethyl sulfoxide (DMSO) solvent was utilized to enhance the properties of the nanostructures under investigation. Solar cell parameters such as the free energy of electron injection ( $\Delta G_{inj}$ ), regeneration ( $\Delta G_{reg}$ ), open-circuit voltage ( $V_{oc}$ ), and light-harvesting efficiency (LHE) were calculated. The results of the photovoltaic parameters indicated that G, SiC, and BN have a high ability to inject electrons into the conduction band minimum (CBM) of titanium dioxide ( $TiO_2$ ) semiconductor. DFT calculations revealed that the HOMO energy levels of the G and SiC nanostructures were localized above the iodine/tri-iodide ( $I/I_3^-$ ) electrolyte, which prevents electrons from regenerating in the ground state. While pristine h-BN exhibits a wide band gap (>6 eV) that limits its utility as a solar sensitizer, our findings reveal that introducing structural defects such as double vacancies or substitutional doping (e.g., h-BN-C) significantly reduces the band gap to values as low as ~2.0 eV. This band gap narrowing enhances the material's ability to absorb visible light and participate in photoinduced charge transfer. Molecular orbital analyses show that the LUMO levels of all defected nanostructures (except h-BN-C in isolated form) lie above the conduction band minimum (CBM) of  $TiO_2$ , enabling efficient electron injection. Furthermore, in the dissolved phase, the HOMO levels of SiC and BN nanostructures shift below the  $I^-/I_3^-$  redox potential, supporting ground-state electron regeneration. TD-DFT results demonstrate pronounced redshift in the UV-Vis absorption spectra of defected and solvated nanostructures, especially for BN-based systems, indicating improved light-harvesting. Overall, this study establishes that through defect engineering and solvent modulation, the optoelectronic performance of 2D materials such as graphene, SiC, and BN can be significantly enhanced, and that defected BN derivatives, once considered unsuitable, emerge as viable sensitizer candidates.

UFS

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# Improved light harvesting with graphene/boron nitride nano-heteroislands: a high-efficiency photosensitizer design

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Density function theory (DFT) and time-dependent density function theory (TD-DFT) are used to deduce the structural, electronic, and optical characteristics of hexagonal boron nitride (h-BN), graphene/boron nitride (G/h-BN), and defected graphene/boron nitride (R-G/h-BN) nanostructures. Furthermore, parameters of solar cell sensitizer devices, such as the free energy of electron injection ( $\Delta G_{inj.}$ ), and regeneration ( $\Delta G_{Reg.}$ ), light harvesting efficiency (LHE), and open circuit voltage (VOC) were computed. Structural calculations revealed the appearance of the Stone–Wales defect when a carbon atom is removed from the center of nanostructures, facilitating faster electron transfer between the nanostructures and the electrolyte. TD-DFT results deduced a red shift in UV–Vis spectrum from ( $\lambda_{max}=213.84$  nm) to ( $\lambda_{max}=372.95$  nm) when graphene structure was placed at the center of h-BN nanostructure and to ( $\lambda_{max}=525.12$  nm) for the R-G/h-BN. The photonic parameter results indicated that the proposed nanostructures exhibited a high ability to inject an electron into the conduction band minimum of the  $TiO_2$  electrode (CBMTiO<sub>2</sub>). Moreover, the LHE results demonstrated that the G/h-BN nanostructure exhibited a stronger response to incident light (LHE=92%) compared to other nanostructures. Furthermore, exhibited ( $\Delta G_{inj.}=-6.646$  eV) a more negative energy compared to ( $\Delta G_{Reg.}=-0.315$  eV). The G/h-BN and h-BN nanoislands have suitable stability compared with natural organic, ruthenium, iridium, and platinum complex dyes. Thus, the investigated nanostructures especially h-BN and G/h-BN hold promise for application in solar cell sensitizer devices.

UFS

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# Indirect probing of light-induced nonadiabatic dynamics in lossy nanocavities

● K. Szabó, Cs. Fábri, G. J. Halász, and Á. Vibók

Light-induced nonadiabatic effects can arise from the interaction of a molecule with the quantized electromagnetic field of a Fabry–Pérot or plasmonic nanocavity. In this context, the quantized radiation field mixes the vibrational, rotational, and electronic degrees of freedom. In this work, we investigate the photodissociation dynamics of a rotating hydrogen molecule within a lossy plasmonic nanocavity. We highlight that, due to significant cavity loss, the dynamics are governed by an infinite number of light-induced conical intersections. We also examine the dissociation dynamics of fixed-in-space molecules by neglecting rotation, employing both the Lindblad master and non-Hermitian lossy Schrödinger equations. Additionally, we incorporate the effects of rotation within the parameter range of perfect agreement using the non-Hermitian lossy Schrödinger method. Furthermore, we show that in the absence of photon losses, there is a close correspondence between the classical Floquet description and the radiation field model.

UFS

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# Impact of dipole self-energy on cavity-induced nonadiabatic dynamics

● Cs. Fábri, G. J. Halász, J. Hofierka, L. S. Cederbaum, and Á. Vibók

The coupling of matter to the quantized electromagnetic field of a plasmonic or optical cavity can be harnessed to modify and control chemical and physical properties of molecules. In optical cavities, a term known as the dipole self-energy (DSE) appears in the Hamiltonian to ensure gauge invariance. The aim of this work is twofold. First, we introduce a method, which has its own merits and complements existing methods, to compute the DSE. Second, we study the impact of the DSE on cavity-induced nonadiabatic dynamics in a realistic system. For that purpose, various matrix elements of the DSE are computed as functions of the nuclear coordinates and the dynamics of the system after laser excitation is investigated. The cavity is known to induce conical intersections between polaritons, which gives rise to substantial nonadiabatic effects. The DSE is shown to slightly affect these light-induced conical intersections and, in particular, break their symmetry.

UFS

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## Controlling molecular dynamics by exciting atoms in a cavity

● A. Csehi, K. Szabó, Á. Vibók, L. C. Cederbaum, and G. J. Halász

Placing an atom and a molecule in a cavity opens the door to initialize molecular dynamics by exciting a level of the atom. This approach enlarges the range of choosing the light source to trigger molecular dynamics substantially. The interplay of the atomic, molecular, and photonic populations gives rise to rich dynamics. The cavity photon plays the role of a mediator between the atom and the molecule and it is found that the photonic population is rather low throughout and its evolution follows that of the molecule. Cavities are known to be subject to losses. In spite of the losses it is demonstrated that the presence of the atom gives rise to a long-lived dynamics that should be of relevance for experimental investigations. The presence of more atoms and molecules is expected to further enrich the dynamics.

UFS

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# Fragmentation in Coulomb explosion of hydrocarbon molecules

● S. S. Taylor, K. Varga, K. Mogyorósi, V. Chikán, and C. Covington

Fragmentation dynamics in the Coulomb explosion of hydrocarbons, specifically methane, ethane, propane, and butane, are investigated using time-dependent density functional theory (TDDFT) simulations. The goal of this work is to elucidate the distribution of fragments generated under laser-driven Coulomb explosion conditions. Detailed analysis reveals the types of fragments formed, their respective charge states, and the optimal laser intensities required for achieving various fragmentations. Our results indicate distinct fragmentation patterns for each hydrocarbon, correlating with the molecular structure and ionization potential. Additionally, we identify the laser parameters that maximize fragmentation efficiency, providing valuable insights for experimental setups. This research advances our understanding of Coulomb explosion mechanisms and offers a foundation for further studies in controlled molecular fragmentation.

**UFS**

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## Light-field-controlled PHz currents in intrinsic metals

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Oriented electric currents in metals are routinely driven by applying an external electric potential. Although the response of electrons to the external electric fields occurs within attoseconds, conventional electronics do not use this speed potential. Ultrashort laser pulses with controlled shapes of electric fields that switch direction at petahertz frequencies open perspectives for driving currents in metals. Light field–driven currents were demonstrated in various media including dielectrics, semiconductors, and topological insulators. Now, our research question is whether we can drive and control orders of magnitude more charge carriers in metals enabling ultrafast switching with practically low-energy, picojoule-level pulses. Here, we demonstrate the interaction of light with nanometer-thick metallic layers, which leads to a generation of light field–controlled electric currents. We show that the implantation of metallic layers into a dielectric matrix leads to up to 40 times increase of the sensitivity in contrast to a bare dielectric, decreasing the intensity threshold for lightwave electronics.

UFS

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# The effect of hydrogen gas and water vapor in catalytic chemical vapor deposition on the structure of vertically aligned carbon nanotubes

● L. Nánai, T. Gyulavári, Zs-R. Tóth, Zs. Pápa, J. Budai, D. Koncz-Horváth, and K. Hernádi

Since the discovery of carbon nanotubes (CNTs), extensive and comprehensive research has been conducted in many areas of materials science. Due to their structural and chemical properties, they can be an important part of electronic devices and structural materials that surround us. In this work, we focused on the preparation and basic analysis of vertically aligned CNTs. An aluminum oxide carrier layer and bimetallic iron–cobalt catalyst layers of different compositions were fabricated on the surface of a silicon substrate using a pulsed laser deposition method. Then, vertically aligned CNTs were grown using a catalytic chemical vapor deposition method based on the thermal decomposition of ethylene. During the experiments, the effect of water vapor and hydrogen gas was investigated on the structure of as-prepared carbon nanotubes. CNT forest samples were characterized by scanning electron microscopy and Raman spectroscopy. One of the most important findings of this research is that the presence of hydrogen gas in the CCVD system is essential, but high-quality vertically aligned CNTs can be produced on silicon substrates even without water vapor.

UFS

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**Materials**  
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# Fabrication of B-C-N nanosheets on Rh(111) from benzene – borazine mixtures

● L. Óvári, G. Vári, A. P. Farkas, M. Farkas, A. Berkó, Gy. Halasi, J. Kiss, N. Oláh, Cs. Vass, and Z. Kónya

Atomic level studies of solid state surfaces performed in ultra-high vacuum (UHV) had already an energetic 15–20 years past when our research group in Szeged started working in this field in mid 1970s. Till then several very important methods had been developed, like UHV technology, commercially available electron and photoelectron spectroscopy techniques, etc. Characterization of metal and semiconductor (oxide) surfaces and their adsorption properties had already been widely studied. In any case, the last 40–50 years also witnessed great discoveries and exciting new techniques. Considering only the activity related to heterogeneous catalysis, the main focus of our research group, new breakthrough methods emerged like HREELS, RAIRS, SPM, NAPXPS, EXAFS, NEXAFS. Along this path, new experimental and theoretical approaches appeared like planar model catalysts and inverse catalysts, atomic level investigation and understanding of surface diffusion-controlled phenomena (particle growth and disruption, strong metal-support interaction (SMSI), decoration, spillover), atomic level identification of active sites, self-organized nano-systems, surface alloys and nanotemplates. It was great to participate in this magical activity for more than 50 years. Both internationally and locally in Szeged, in the last two decades, surface science has opened to the wide world of 2D materials like the semimetal graphene and the insulator hexagonal boron nitride. However, the formation of a mixed layer of C, B and N proved to be a difficult task due to the primary tendency for phase separation. In the present work, we report on a preparation method of honeycomb “BCN” materials on Rh(111) by using benzene/borazine mixtures as precursors. It was demonstrated that by a suitable choice of the growth parameters, the formation of large, separated graphene and h-BN islands can be avoided.

UFS, Eng

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# CH(A) radical formation in Coulomb explosion from butane seeded plasma generated with chirp-controlled ultrashort laser pulses

● K. Mogyorósi, B. Tóth, K. Sárosi, B. Gilicze, J. Csontos, T. Somoskői, Sz.Tóth, P. P. Geetha, L. Tóth, S. S. Taylor, N. Skoufis, L. Barron, K. Varga, C. Covington and V. Chikán

We experimentally studied the formation of CH(A) radicals in butane seeded plasma generated with chirp-controlled ultrashort laser pulses ( $\sim 760 \mu\text{J/pulse}$ ,  $890 \text{ nm}$ ,  $1 \text{ kHz}$ ,  $8 \text{ fs}$ ). The focused beam with high peak intensity ( $\sim 10^{14} - 10^{16} \text{ W/cm}^2$ ) caused Coulomb explosion (CE). The time-dependent emission spectra were observed with the Fourier-transform Visible spectroscopy (FTVis) step-scan method. The average signal intensity decreased with the chirp in the  $\text{Ar}^+ > \text{C}_2 > \text{H-}\alpha \sim \text{CH(A)}$  order, with a plateau for CH(A) in the  $-200$  to  $-100 \text{ fs}^2$  range. The short rise time of the CH(A) emission signal, the monoexponential emission decay and the nearly constant rotational and vibrational temperatures of the CH(A) radicals ( $\sim 3000$  and  $\sim 3800 \text{ K}$ ) all support their potential formation as a primary product ( $< 120 \text{ fs}$ ) or in other photodissociation, neutralization processes before collisions of the fragments ( $< 2 \text{ ns}$ ). Our TDDFT calculations predict that CH and many other fragments can be formed beyond CE at  $\sim 7 \times 10^{14} \text{ W/cm}^2$  intensity. The average charge of CH ( $+0.6$ ) and its relative abundance ( $0.5\%$ ) support the formation of detectable CH(A) within  $120 \text{ fs}$ . Suitable optical gating techniques and measurement of the temporal evolution of the electron density in plasma could elucidate the relative importance of the different formation pathways of the CH(A) radicals in the first nanosecond after CE.

## UFS

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# A comparative study of femtosecond pulsed and continuous wave lasers on physiological responses through activation of phytochromes in seeds

● Cs. M. Szabó, B. Bán, B. Sinka, B. Tóth, B. Gilicze, I. Seres, J. Bohus, A. Ébert, P. Borbély, Zs. Gulyás, G. Galiba, E. Darko, M. Hovári, B. Hopp, Cs. Péter, K. Mogyorósi, and A. Viczián

Red light activates phytochrome photoreceptors, which mediate such key developmental steps as germination and seedling photomorphogenesis in *Arabidopsis thaliana*. To examine the details of these responses, we developed a novel experimental system and demonstrated that brief, high-intensity light pulses can elicit sustained physiological responses. We observed that the seeds responded to the femtosecond laser light pulses, but with lower sensitivity compared with continuous light sources having the same average fluence. We concluded that (i) phytochrome B photoreceptors within imbibed seeds efficiently absorb red and far-red photons from pulsed femtosecond laser pulses, with absorption occurring during approximately 10 orders of magnitude shorter amount of time than with conventional light sources; (ii) these treatments did not induce adverse effects during later plant development; and (iii) the effect of ultrashort light pulses in planta coincides with phytochrome photoconversion characteristics described during in vitro studies. Our findings demonstrate that seed germination and photomorphogenic development can be effectively triggered by light, regardless of whether it is delivered continuously or within extremely brief pulses. This research expands the potential applications of femtosecond laser technology and demonstrates the feasibility of investigating the effects of ultrafast physical phenomena on biological processes in vivo using diverse biological readouts.

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**Scientific Reports**  
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# Electrochemical modulation of hole extraction in NiO/perovskite bilayers

● X. Chen, K. Sárosi, B. Tóth, B. Gilicze, Zs. Bengery, K. Mogyorósi, Cs. Janáky, and G. F. Samu

Charge extraction (or injection) at the transport layer/lead halide perovskite interface is a decisive process in determining the efficiency of optoelectronic devices. To elucidate the influence of band offsets on the hole transfer process, a series of perovskite thin films with systematically tuned valence band positions ( $\text{FA}_{0.83}\text{Cs}_{0.17}\text{Pb}(\text{I}_{1-x}\text{Br}_x)_3$ ) are fabricated and deposited on mesoporous NiO hole transport layers. In this work, transient absorption spectroscopy is performed to study the kinetics of hole transfer through the NiO/perovskite interface. It is revealed that a larger valence band offset is beneficial for hole extraction. To understand how hole depletion/accumulation influences the hole extraction process, in situ transient spectroelectrochemical measurements are also employed. These results highlight that, at negative applied electrochemical biases, an acceleration of the hole transfer process is found for different perovskite compositions. A more pronounced increase in the hole extraction rate can be tied to a larger valence band offset at the NiO/perovskite interface. These results provide a better understanding of the charge extraction process at NiO/perovskite interfaces, enabling more rational design of these systems.

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# Highly sensitive detection of the hazardous insecticide carbofuran using tungsten disulfide nanosheets decorated with gold nanoparticles

● V. S. Haritha, S. R. Sarath Kumar, and R. B. Rakhi

The present study explores the development of an advanced electrochemical sensor designed to detect and quantify a carbamate pesticide, carbofuran (CB), using gold nanoparticles decorated tungsten disulphide nanosheets (Au-WS<sub>2</sub>). Au nanoparticles have been integrated into the WS<sub>2</sub> nanosheets through an in-situ chemical reduction method. The sensors made with Au-WS<sub>2</sub> exhibit significantly improved performance compared to the pristine WS<sub>2</sub> nanosheets. The addition of Au nanoparticles alters the surface properties of the electrode, increasing the number of active sites for electrochemical reactions and enhancing electron transfer properties, even with a small atomic fraction of Au (<10 %) in the WS<sub>2</sub> nanosheets. The Au-WS<sub>2</sub> modified electrode demonstrates superior sensitivity (2.83  $\mu\text{A } \mu\text{M}^{-1} \text{cm}^{-2}$ ) and selectivity compared to WS<sub>2</sub> nanosheets in detecting carbofuran offering a lower detection limit of 0.09  $\mu\text{M}$ . Evaluation of the reproducibility and the stability of the fabricated sensor reveal consistent performance over longer periods. The fabricated Au-WS<sub>2</sub> CB sensor exhibits promising potential for practical applications in environmental monitoring and food safety.

IA

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# Modelling of tiled grating arrangement efficiency

● V. S. Haritha, G. Horváth, and M. Füle

The precise alignment of individual diffraction grating units within a tiled grating assembly (TGA) is essential for enhancing the quality of optical throughput and overall functional performance of such kinds of optical systems. This study presents a comprehensive simulation analysis of TGAs comprising two and four gratings to assess the sensitivity of optical imaging performance to a range of induced alignment errors. The misalignments are systematically introduced to the grating sections in the tiled grating assemblies, and their effects in far-field imaging are examined and compared. The results highlight the critical role of accurate alignment in maintaining coherent beam combination and optimal system performance. Zemax OpticStudio®-based simulations offer valuable insights for designing high-performance, large-aperture grating systems and pave the way for future experimental validation and integration.

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# Towards a new vision of PaNET: enhancing reasoning capabilities for better photon and neutron data discovery

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The Photon and Neutron Experimental Techniques (PaNET) ontology was released in 2021 as an ontology for two major European research infrastructure communities. It provides a standardized taxonomy of experimental techniques employed across the photon and neutron scientific domain, and is part of a wider effort to apply the FAIR (findable, accessible, interoperable, reusable) principles within the community. Specifically, it is used to enhance the quality of metadata in photon and neutron data catalogue services. However, PaNET currently relies on a manual definition approach, which is time consuming and incomplete. A new structure of PaNET is proposed to address this by including logical frameworks that enable automatic reasoning as opposed to the manual approach in the original ontology, resulting in over a hundred new technique subclass relationships that are currently missing in PaNET. These new relationships, which are evaluated by the PaNET working group and other domain experts, will improve data catalogue searches by connecting users to more relevant datasets, thereby enhancing data discoverability. In addition, the results of this work serve as a validation mechanism for PaNET, as the very process of building the logical frameworks, as well as any incorrect inferences made by the reasoner, has exposed existing issues within the original ontology.

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