ABSTRACTS

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A comparative study of femtosecond pulsed laser ablation of meloxicam in distilled water and in air

E. Nagy, J. Kopniczky, T. Smausz, M. Náfrádi, T. Alapi, J. Bohus, V. Pajer, P. Szabó-Révész, R. Ambrus, and B. Hopp

The increasing prevalence of water insoluble or poorly soluble drugs calls for the development of new formulation methods. Common approaches include the reduction of particle size and degree of crystallinity. Pulsed laser ablation is a clean technique for producing sub-micrometre sized drug particles and has the potential to induce amorphization. We studied the effect of femtosecond pulsed laser ablation (ELI ALPS THz pump laser system: λc=781 nm, τ=135 fs) on meloxicam in distilled waterand in air. The ablated particles were characterized chemically, morphologically and in terms of crystallinity. We demonstrated that femtosecond laser ablation can induce partial amorphization of the particles in addition to a reduction in particle size. In the case of femtosecond pulsed laser ablation in air, the formation of pure meloxicam spheres showed that this technique can produce amorphous meloxicam without the use of excipients, which is a unique result. We also aimed to describe the ablation processes in both investigated media.

LaSo

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Single thin-plate compression of multi-TW laser pulses to 3.9 fs

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Post-compression of 12-fs laser pulses with multi-TW peak power from an optical parametric chirped pulse amplification (OPCPA) system was performed by using a single thin fused silica plate in a vacuum. By optimizing the input pulses in both spatial and temporal domains, after compression with customized chirped mirrors, we achieved pulses as short as 3.87 fs, in combination with 12-mJ energy. The spatio-spectral quality of the post-compressed pulses was thoroughly analyzed. The generated 1.4-cycle pulses pave the way for next generation attosecond and particle acceleration experiments.

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Spectrally tunable ultrashort monochromatized extreme ultraviolet pulses at 100 kHz

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We present the experimental realization of spectrally tunable, ultrashort, quasi-monochromatic extreme ultraviolet (XUV) pulses generated at 100 kHz repetition rate in a user-oriented gas high harmonic generation beamline of the Extreme Light Infrastructure—Attosecond Light Pulse Source facility. Versatile spectral and temporal shaping of the XUV pulses is accomplished with a double-grating, time-delay compensated monochromator accommodating the two composing stages in a novel, asymmetrical geometry. This configuration supports the achievement of high monochromatic XUV flux ($2.8 \pm 0.9 \times 10^{10}$ photons/s at 39.7 eV selected with 700 meV full width at half maximum bandwidth) combined with ultrashort pulse duration (4.0 ± 0.2 fs using 12.1 ± 0.6 fs driving pulses) and small spot size (sub-100 μm). Focusability, spectral bandwidth, and overall photon flux of the produced radiation were investigated, covering a wide range of instrumental configurations. Moreover, complete temporal (intensity and phase) characterization of the few-femtosecond monochromatic XUV pulses—a goal that is difficult to achieve by conventional reconstruction techniques—has been realized using a ptychographic algorithm on experimentally recorded XUV-infrared pump–probe traces. The presented results contribute to in situ, time-resolved experiments, accessing direct information on the electronic structure dynamics of novel target materials.

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Ion acceleration with few cycle relativistic laser pulses from foil targets

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Ion acceleration resulting from the interaction of 11 fs laser pulses of ~35 mJ energy with ultrahigh contrast ($<10^{-10}$) and 10^{19} W cm^{-2} peak intensity with foil targets made of various materials and thicknesses at normal (0°) and 45° laser incidence is investigated. The maximum energy of the protons reached 1.4 MeV accelerated in the laser propagation direction and 1.2 MeV in the opposite direction from a formvar target. The energy conversion efficiency from the laser to the proton beam is estimated to be as high as 1.4% at 45° laser incidence using a 51 nm thick Al target. The high laser contrast indicates the predominance of vacuum heating via Brunel's effect as an absorption mechanism involving a tiny pre-plasma at the target front. The experimental results are in reasonable agreement with theoretical estimates, where proton acceleration from the target front side in the backward direction is well explained by the Coulomb explosion of a charged cavity formed in a tiny pre-plasma, while forward proton acceleration is likely to be a two-step process: protons are first accelerated in the target front-side cavity and then further boosted in energy through the target back side via the target normal sheath acceleration (TNSA) mechanism.

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High-order harmonic generation in a strongly overdriven regime

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High-order harmonic generation (HHG) normally requires a careful adjustment of the driving laser intensity (typically 10^{14}–10^{15} W/cm^2) and gas medium parameters to obtain a microscopically and macroscopically optimized output. In contrast to conventional wisdom, we present experimental results indicating efficient HHG in all rare gases, using a high-density medium and a driving laser intensity of around 10^{16} W/cm^2. The experimental results are corroborated by theoretical simulations, which indicate that ionization-induced self-phase modulation and plasma defocusing self-regulate the driver laser intensity to a level that allows efficient HHG. A tenfold broadening of the driving near-infrared spectrum is observed, which results in the generation of continuous spectra from 18 to 140 eV in spite of using 50-fs-long driving pulses. The presented scheme represents a simple and versatile concept for the generation of extreme-ultraviolet and soft-x-ray continua, which could be used for transient absorption and reflection spectroscopy.

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Quantum electrodynamics of ultra-intense laser-matter interactions

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Intense laser-matter interactions are at the center of interest in research and technology since the development of high-power lasers. They have been widely used for fundamental studies in atomic, molecular, and optical physics, and they are at the core of attosecond physics and ultrafast optoelectronics. Although the majority of these studies have been successfully described using classical electromagnetic fields, recent investigations based on fully quantized approaches have shown that intense laser-atom interactions can be used for the generation of controllable high-photon-number entangled coherent states and coherent state superpositions. In this tutorial, we provide a comprehensive fully quantized description of intense laser-atom interactions. We elaborate on the processes of high-harmonic generation, above-threshold ionization, and we discuss new phenomena that cannot be revealed within the context of semiclassical theories. We provide the description for conditioning the light field on different electronic processes, and their consequences for quantum state engineering of light. Finally, we discuss the extension of the approach to more complex materials, and the impact to quantum technologies for a new photonic platform composed of the symbiosis of attosecond physics and quantum information science.

SeSo

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Squeezed light effect

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The interaction of atoms with intense squeezed light is affected by the quantum noise of the driving field whereby the quantum noise of the squeezed driving field is imprinted in the emitted high harmonics.

SeSo
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Strong–laser–field physics, non–classical light states and quantum information science

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Strong–laser–field physics is a research direction that relies on the use of high-power lasers and has led to fascinating achievements ranging from relativistic particle acceleration to attosecond science. On the other hand, quantum optics has been built on the use of low photon number sources and has opened the way for groundbreaking discoveries in quantum technology, advancing investigations ranging from fundamental tests of quantum theory to quantum information processing. Despite the tremendous progress, until recently these directions have remained disconnected. This is because the majority of the interactions in the strong-field limit have been successfully described by semi-classical approximations treating the electromagnetic field classically, as there was no need to include the quantum properties of the field to explain the observations. The link between strong–laser–field physics, quantum optics, and quantum information science has been developed in the recent past. Studies based on fully quantized and conditioning approaches have shown that intense laser–matter interactions can be used for the generation of controllable entangled and non-classical light states. These achievements open the way for a vast number of investigations stemming from the symbiosis of strong–laser–field physics, quantum optics, and quantum information science. Here, after an introduction to the fundamentals of these research directions, we report on the recent progress in the fully quantized description of intense laser–matter interaction and the methods that have been developed for the generation of non-classical light states and entangled states. Also, we discuss the future directions of non-classical light engineering using strong laser fields, and the potential applications in ultrafast and quantum information science.

SeSo

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Generation of micro-Joule level coherent quasi-continuum extreme ultraviolet radiation using multi-cycle intense laser-atom interactions

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In the present work we report on the current progress of the recently constructed GW attosecond extreme ultraviolet (XUV) source developed at the Institute of Electronic Structure and Laser of the Foundation for Research and Technology-Hellas (I.E.S.L-FO.R.T.H.). By the implementation of a compact-collinear polarization gating arrangement, the generation of a broadband, coherent XUV quasi-continuum produced by the interaction of a many-cycle infrared field with a gas phase medium is achieved. The spectral width of the XUV emission generated in Xenon, is spanning in the range of 17–32 eV and can support isolated pulses of duration in the range from 0.4 fs to 1.3 fs and pulse energy in the 1 μJ level. Theoretical calculations, taking into account the experimental conditions of this work, are supporting the observations, offering also an insight regarding the temporal profile of the emitted radiation. Finally, the high intensity of the produced XUV pulses has been confirmed by investigating the two-XUV-photon double ionization process of Argon atoms. The demonstrated results inaugurate the capability of the beamline of producing intense coherent quasi-continuum XUV radiation, supporting isolated as pulses, that can be exploited in studies of non-linear XUV processes, attosecond pulse metrology and XUV-pump–XUV-probe experiments.

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Numerical representation of tightly focused ultra-short laser pulses

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A scheme for numerical representation for the fields of tightly focused laser pulses is presented going beyond the paraxial framework that gives accurate values up to near single-cycle pulses. The laser field is defined by a solution of the paraxial Helmholtz equation and a temporal pulse profile in light-cone coordinates, the fourth- and second-order corrections are provided for short pulses and vector beams, and the absolute error of these terms is presented. The method can give an accurate field description for any transverse electromagnetic mode, and it is suited for providing initial fields for existing solvers for Maxwell's equations, such as in the particle-in-cell codes.

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Hybrid acceleration of compact ion bunches by few-cycle laser pulses in gas jets of two atomic species

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Extreme states of matter that exist for a short time need probing with compact proton sources. Here, the generation of a compact MeV-energy proton source from few-cycle laser pulse interaction with narrow gas-jet target is demonstrated numerically. We realize such proton source by incorporating a gas mixture which is optimal for generation of quasimonoenergetic proton bunches. In the presented laser-plasma interaction we identify the ion acceleration from magnetic vortex, charge separation, and collisionless shock wave. The proposed particle source is excellent for applications where moderate-energy proton bunches are used at high repetition rate. We prove the applicability of this scheme for generating a pulsed spherical neutron burst with ~100 ps duration.

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Three-stage laser wakefield accelerator scheme for sub-Joule few-cycle laser pulses

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Laser-driven electron acceleration in underdense plasma is a promising route towards the realization of reliable sources of relativistic electrons in the 0.1–1 GeV energy range. Generation of such electron bunches at high repetition rates is hindered by the limited energy per pulse, which inevitably results in very short pulse duration and tight focusing. Compressing the laser energy in time and space allows scientists to use higher plasma density to drive wakefieds, which in turn results in enhanced diffraction and dispersion of the broadband laser pulse. These features make difficult to control the acceleration in the plasma wave and to improve the beam quality. Here we propose a mm-long three-stage acceleration scheme, which allows for tunable injection and optimal acceleration of high-quality electron bunches. The full interaction length is modeled by 3D particle-in-cell simulations.

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Controlled transition to different proton acceleration regimes: Near-critical-density plasmas driven by circularly polarized few-cycle pulses

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A controlled transition between two different ion acceleration mechanisms would pave the way to achieving different ion energies and spectral features within the same experimental set up, depending on the region of operation. Based on numerical simulations conducted over a wide range of experimentally achievable parameter space, reported here is a comprehensive investigation of the different facets of ion acceleration by relativistically intense circularly polarized laser pulses interacting with thin near-critical-density plasma targets. The results show that the plasma thickness, exponential density gradient, and laser frequency chirp can be controlled to switch the interaction from the transparent operating regime to the opaque one, thereby enabling the choice of a Maxwellian-like ion energy distribution with a cutoff energy in the relativistically transparent regime or a quasi-monoenergetic spectrum in the opaque regime. Next, it is established that a multispecies target configuration can be used effectively for optimal generation of quasi-monoenergetic ion bunches of a desired species. Finally, the feasibility is demonstrated for generating monoenergetic proton beams with energy peak at E≈20–40 MeV and a narrow energy spread of ΔE/E≈18%–28.6% confined within a divergence angle of 175 mrad at a reasonable laser peak intensity of I_0 5.4 × 10^{20} W/cm^2.

SeSo

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Photo-ionization initiated differential ultrafast charge migration: impact of molecular symmetries and tautomeric forms

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Photo-ionization induced ultrafast electron dynamics is considered as a precursor for the slower nuclear dynamics associated with molecular dissociation. Here, using the ab initio multielectron wave-packet propagation method, we study the overall many-electron dynamics, triggered by ionizing the outer-valence orbitals of different tautomers for a prototype molecule with more than one symmetry element. From the time evolution of the initially created averaged hole density of each system, we identify distinctly different charge dynamics responses in the tautomers. We observe that the keto form shows a charge migration direction away from the nitrogen bonded with hydrogen, while in enol–U – away from oxygen bonded to hydrogen. Additionally, the dynamics following the ionization of molecular orbitals with different symmetries reveals that a′ orbitals show a fast and highly delocalized charge density in comparison to a′′ symmetry. These observations indicate why different tautomers respond differently to an XUV ionization,and might explain the subsequent different fragmentation pathways. An experimental schematics allowing the detection and reconstruction of such charge dynamics is also proposed. Although the present study uses a simple, prototypical bio-relevant molecule, it reveals the explicit role of molecular symmetry and tautomerism in the ionization-triggered charge migration that controls many ultrafast physical, chemical, and biological processes, making tautomeric forms a promising tool of molecular design for desired charge migration.

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Atomic scale interfacial magnetism and origin of metal-insulator transition in $(LaNiO_3)_n/(CaMnO_3)_m$ superlattices: a first principles study

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Interfacial magnetism and metal-insulator transition at $LaNiO_3$-based oxide interfaces have triggered intense research efforts, because of the possible implications in future heterostructure device design and engineering. Experimental observation lack in some points a support from an atomistic view. In an effort to fill such gap, we hereby investigate the structural, electronic, and magnetic properties of $(LaNiO_3)_n/(CaMnO_3)_m$ superlattices with varying $LaNiO_3$ thickness (n) using density functional theory including a Hubbard-type effective on-site Coulomb term. We successfully capture and explain the metal-insulator transition and interfacial magnetic properties, such as magnetic alignments and induced Ni magnetic moments which were recently observed experimentally in nickelate-based heterostructures. In the superlattices modeled in our study, an insulating state is found for n=1 and a metallic character for n=2, 4, with major contribution from Ni and Mn 3d states. The insulating character originates from the disorder effect induced by sudden environment change for the octahedra at the interface, and associated to localized electronic states; on the other hand, for larger n, less localized interfacial states and increased polarity of the $LaNiO_3$ layers contribute to metallicity. We discuss how the interplay between double and super-exchange interaction via complex structural and charge redistributions results in interfacial magnetism. While $(LaNiO_3)_n/(CaMnO_3)_m$ superlattices are chosen as prototype and for their experimental feasibility, our approach is generally applicable to understand the intricate roles of interfacial states and exchange mechanism between magnetic ions towards the overall response of a magnetic interface or superlattice.

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Inorganic drugs as a tool for protein structure solving and studies on conformational changes

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Inorganic drugs are capable of tight interactions with proteins through coordination towards aminoacidic residues, and this feature is recognized as a key aspect for their pharmacological action. However, the “protein metalation process” is exploitable for solving the phase problem and structural resolution. In fact, the use of inorganic drugs bearing specific metal centers and ligands capable to drive the binding towards the desired portions of the protein target could represent a very intriguing and fruitful strategy. In this context, a theoretical approach may further contribute to solve protein structures and their refinement. Here, we delineate the main features of a reliable experimental-theoretical integrated approach, based on the use of metallodrugs, for protein structure solving.

US

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Effect of reduced graphene oxide hybridization on ZnO nanoparticles sensitivity to NO_2 gas: A DFT study

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In the present work, a density functional theory (DFT) calculation to simulate reduced graphene oxide (rGO) hybrid with zinc oxide (ZnO) nanoparticle's sensitivity to NO_2 gas is performed. In comparison with the experiment, DFT calculations give acceptable results to available bond lengths, lattice parameters, X-ray photoelectron spectroscopy (XPS), energy gaps, Gibbs free energy, enthalpy, entropy, etc. to ZnO, rGO, and ZnO/rGO hybrid. ZnO and rGO show n-type and p-type semiconductor behavior, respectively. The formed p-n heterojunction between rGO and ZnO is of the staggering gap type. Results show that rGO increases the sensitivity of ZnO to NO_2 gas as they form a hybrid. ZnO/rGO hybrid has a higher number of vacancies that can be used to attract oxygen atoms from NO_2 and change the resistivity of the hybrid. The combined reduction of oxygen from NO_2 and NO can give a very high value of the Gibbs free energy of reaction that explains the ppb level sensitivity of the ZnO/rGO hybrid. The dissociation of NO_2 in the air reduces the sensitivity of the ZnO/rGO hybrid at temperatures higher than 300˚C.

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Decisive role of Cu/Co interfaces in copper cobaltite derivatives for high performance CO_2 methanation catalyst

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Thermo-catalytic bio-SNG (CH_4) production is one of the useful tools for converting waste to gaseous fuels through CO_2 conversion. To abundant properly, however, efficient, robust and cost-effective catalysts would be required. Bimetallic systems based on transition metals seem to be promising candidates for this task. The CoCu bimetallic system with in-situ generated interfaces was synthesized and used as a catalyst for CO_2 methanation. The in-depth analysis of the structure-activity-selectivity relationships involving XRD, (NAP-)XPS, EXAFS and TEM-EDX revealed that the co-existence of Co^0, CoO, and Cu^0 in the proper distribution on the surface can ensure the selective production of methane. To fine-tune the surface composition of the bimetallic systems, a systematic alteration of the Cu:Co ratio in the precursor spinel structures must be performed. $Cu_{0.4}Co_{2.6}O_4$ derivative, stabilizing subsurface Cu(I)–O specimen, showed the best performance with high activity (12,800 nmol g^{-1} s^{-1}) and a remarkable selectivity of 65–85% for methane in a wide temperature range (250–425 °C). In studying the mechanistic aspects of methanation, it has been shown that the hydrogenation of active carbon at the surface or below the surface is the key step for the production of methane. So far, this cobalt-catalyzed sub-step has been proposed in catalytic Fischer-Tropsch syntheses.

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New insights into thermal processes of metal deposits on h-BN/Rh(1 1 1): A comparison of Au and Rh

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In this paper the thermal properties of Au and Rh deposits are compared on hexagonal boron nitride (h-BN) “nanomesh” prepared on Rh(111), applying STM, XPS, low energy ion scattering (LEIS), LEED, and DFT. At room temperature, both metals essentially follow Volmer-Weber (3D) growth. Upon subsequent annealing, agglomeration (sintering), intercalation, and desorption are competing surface processes for both metals. For the more reactive Rh, we suggest an additional encapsulation mechanism: between 600 K and 750 K, fragments of decomposed h-BN diffuse locally from the bottom onto the metal clusters covering them partially. STM data indicates that agglomeration of gold nanoparticles proceeds faster compared to rhodium. At higher temperatures (1050 K–1100 K), all non-desorbing gold atoms diffuse below h-BN, even for large initial coverages. On the other hand, for larger Rh deposits (≥5 ML), the outermost layer always contains Rh. Accumulation of gold at the interface between h-BN and Rh(111) significantly enhances the thermal stability of h-BN, attributed to the lower reactivity of Au in the decomposition of h-BN compared to Rh(111). At elevated substrate temperatures, intercalation of individual adatoms takes place during deposition, which requires higher temperatures for rhodium due to its slower diffusion and higher probability of nucleation.

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Local hydrophobicity allows high-performance electrochemical carbon monoxide reduction to C_{2+} products

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While CO can already be produced at industrially relevant current densities via CO_2 electrolysis, the selective formation of C_{2+} products seems challenging. CO electrolysis, in principle, can overcome this barrier, hence forming valuable chemicals from CO_2 in two steps. Here we demonstrate that a mass-produced, commercially available polymeric pore sealer can be used as a catalyst binder, ensuring high rate and selective CO reduction. We achieved above 70% faradaic efficiency for C_{2+} products formation at j = 500 mA cm^{-2} current density. As no specific interaction between the polymer and the CO reactant was found, we attribute the stable and selective operation of the electrolyzer cell to the controlled wetting of the catalyst layer due to the homogeneous polymer coating on the catalyst particles' surface. These results indicate that sophistically designed surface modifiers are not necessarily required for CO electrolysis, but a simpler alternative can in some cases lead to the same reaction rate, selectivity and energy efficiency; hence the capital costs can be significantly decreased.

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Diatomic molecule in a strong infrared laser field: level-shifts and bond-length change due to laser-dressed Morse potential

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We present a general mathematical procedure to handle interactions described by a Morse potential in the presence of a strong harmonic excitation. We account for permanent and field-induced terms and their gradients in the dipole moment function, and we derive analytic formulae for the bond-length change and for the shifted energy eigenvalues of the vibrations, by using the Kramers–Henneberger frame. We apply these results to the important cases of H_2 and LiH, driven by a near- or mid-infrared laser in the $10^{13}\,\mathrm{W\,cm^{-2}}$ intensity range.

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