ABSTRACTS



Laser-based QR code marking on double film-coated tablets: balancing marking efficiency and tablet integrity — a step toward safer medicines

H. Shammout, B. Hopp, T. Smausz, J. Bohus, O. Jójárt, Laczkovich, M. Cseh, J. Kopniczky, B. Tari, R. Saker, K. Kristó, T. Sovány, and K. Ludasi

Background/Objectives: Laser has a prominent place in pharmaceutical industry, especially in the marking of solid dosage forms (SDFs). To combat falsified medicines, this study evaluates QR code marking on the surface of tablets as a supplement to serialization on packaging, using an ultrafast laser to achieve industrially relevant marking speeds while preserving the functional integrity of double film-coated ibuprofen tablets. Methods: Tablets were directly compressed and coated with a double film: the inner layer was a gastro-resistant coating (Acryl-EZE® MP), while the outer one was a coloured, TiO_2-containing (TC) or TiO_2-free (TF) immediate-release coating (Opadry®). QR codes were ablated on the tablet surface using various laser parameters (e.g., pulse energy and scanning speed), and the effects were physically, chemically, and microscopically examined to evaluate their properties after this processing. Results: No significant differences were observed between TC and TF coatings. In addition, the readability of QR code is strongly influenced by laser settings and coating types. Furthermore, the used laser has achieved the expected fast marking speed and high-precision coding, which may be economically feasible for pharmaceutical companies. According to the profilometry findings, the ablation depth could be compensated for with an appropriate coating thickness to enable the desired release properties. This was confirmed by the results of SEM, Raman analysis, and in vitro dissolution test. Conclusions: Ultrafast Ti:Sa laser-based QR code marking directly onto the dosage form offers increasing benefits in the healthcare field. However, it may undesirably affect the behavior of the dosage form. This requires careful consideration of formulation and laser processing conditions before application, especially in the case of delayed-release (DR) systems.

LaSo

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Pharmaceutics
18 (2026) 1, 73

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Investigation of the photoprotective effects of various pigments against laser-marking of pharmaceutical tablets

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Background/Objectives: With the increasing incidence of drug counterfeiting and the emergence of personalized medicine, the need for unique marking of solid dosage forms, e.g., tablets, has attracted considerable interest in the current research and development landscape. Besides traditional printing methods, laser marking offers several advantages, as it eliminates the need for organic solvents and enables the generation of precise patterns. However, laser exposure may raise safety concerns regarding the stability of photosensitive drugs in the irradiated dosage forms. Therefore, the aim of the present study was to test the photoprotective effect of titanium dioxide (TiO_2) and its various alternatives, e.g., talc, calcium carbonate ($CaCO_3$), zinc oxide (ZnO), and black iron oxide (Fe_3O_4), alongside a ready-to-use reference formulation, Opadry® Brown, which contains TiO_2 (titanium-containing, TC) on nifedipine, a light-sensitive model drug. Methods: Laser marking or short-term laser ablation at different wavelengths (193 nm, 248 nm, 532 nm, and 781 nm) was applied to different coating formulations. As a positive control, prolonged exposure to daylight was applied. The properties and photostability of these formulations were evaluated using several analytical methods (i.e., surface profilometry, Raman spectroscopy, and high-performance liquid chromatography (HPLC)). Results: The TiO_2, ZnO, Fe_3O_4, and Opadry® TC Brown coatings maintained their color during the long-term study under all conditions. Furthermore, the prepared formulations exhibited different ablation depths and morphological changes depending on the coating and laser type. HPLC measurements confirmed significant differences in the protective ability of various pigments against sunlight and different types of lasers. Nevertheless, the obtained Raman spectra were not in complete agreement with HPLC results, which can be attributed to spectral overlap between key nifedipine degradation markers and excipient signals in the tablet core. Conclusions: Overall, laser treatment of tablets containing photosensitive drugs may induce API decomposition; however, this effect can be minimized or avoided by careful selection of the appropriate combination of laser type and photoprotective pigment. Under the applied experimental conditions, Ti:Sa laser treatment was associated with the lowest degree of nifedipine degradation among all formulations, while ZnO-containing coatings demonstrated the most consistent photoprotective performance against the majority of the tested laser types, while Fe_3O_4-containing coatings provided superior protection during prolonged sunlight exposure and Nd:YAG laser irradiation.

LaSo

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Pharmaceutics
18 (2026) 6, 758

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Over 400 W average power, sub-two-cycle, carrier-envelope phase-stable fiber laser system

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We report on the development of a carrier-envelope phase (CEP)-stable 1030 nm fiber-based laser system producing 6.2 fs pulses achieved via the multi-pass cell (MPC) post-compression technique with 402 W average power at 100 kHz repetition rate. This system employs an upgraded three-stage MPC compression scheme exhibiting excellent beam quality properties for this intensity region. Active stabilization locks the CEP noise below 430 mrad root mean square. This work represents the first demonstration of a coherently combined fiber laser system simultaneously achieving such exceptional average power, CEP stability and sub-two-cycle pulse durations. Similar to all other light sources of the Extreme Light Infrastructure Attosecond Light Pulse Source, this newly developed system is accessible to the international research community in peer-reviewed open user calls of the Extreme Light Infrastructure European Research Infrastructure Consortium.

LaSo

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High Power Laser Science and Engineering 14 (2026) e11

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Single-cycle mid-infrared pulses with 30 µJ at 100 kHz via post-compression in solid-state media

R. Shrestha, L. Lehotai, R. S. Nagymihály, K. Pirisi, Á. Börzsönyi, E. Cormier, and B. Kiss

We demonstrate a 3.2 µm mid-infrared source delivering 30 µJ, single-cycle pulses via two-stage bulk post-compression of a 10 W four-cycle OPCPA. By optimizing a tandem configuration of BaF_2 and Si, we achieved a compressed pulse duration of 11 fs with a CEP stability of 145 mrad RMS. The output exhibited high spatio-spectral uniformity with small residual spatial and angular chirp. The reliability and long-term stability of the system are tested. Additionally, high-order harmonics were generated in ZnO with locked CEP. The demonstrated performance is ideal for strong-field and attosecond-science applications.

LaSo

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Optics Letters
51 (2026) 11

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Spatially and temporally resolved simulation of high-energy post-compression in thin dielectric plates

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As we progress towards the limits of modern, high-peak power chirped pulse amplification in terms of gain bandwidth, various post-compression techniques are emerging to further shorten the duration of these pulses. Here, we present a spatio-temporally resolved simulation environment for the post-compression of energetic ultrashort laser pulses in thin dielectric media. Our approach applies an advanced Fourier transform technique, which helps to reduce computational costs drastically. We also provide experimental validation to support our simulations. In addition to showing excellent agreement with measured data from multi-TW, single-cycle post-compression experiments, the theoretical results revealed complex spatio-spectral and spatio-temporal features. The developed platform enables robust a priori optimization of post-compression setups across a broad energy range, from tens of millijoules to tens of Joules.

LaSo

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Optics Express
34 (2026) 13, 23314-23328

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Ultrahigh contrast petawatt laser with a mJ-class femtosecond parametric seeder for high repetition rate experiments

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A novel, to the best of our knowledge, millijoule-class femtosecond optical parametric amplification-based source is implemented as a seeder in the high-repetition-rate HF-PW laser of ELI ALPS. High energy seeding results in a bandwidth corresponding to a sub-19 fs transform limit, significant gain reduction in the Ti:Sa amplifier chain, and an extremely low amplified spontaneous emission relative intensity of 2×10^{-14} with 10 J compressed energy. The combination of the achieved parameters with the routinely available 2.5 or 5 Hz repetition rate offers unprecedented opportunities for the generation of particles and high harmonics.

LaSo

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Optics Letters
51 (2026) 13, 3789-3792

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Helium-enhanced spectral broadening in CO_2-filled hollow-core fiber

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We demonstrate enhanced spectral broadening of femtosecond pulses (330 fs, 1030 nm, 5–200 kHz) in a hollow-core fiber (HCF) using CO_2/helium gas mixtures. While increasing pure CO_2 pressure broadens the spectrum and induces a Raman redshift, it causes substantial optical loss. Introducing a helium buffer enables strong broadening at reduced CO_2 pressures, significantly decreasing loss. Propagating pulses through a 1-m-long, 300-μm-core HCF, we show that helium enhances spectral width, extends the Raman shift, and improves transmitted power by facilitating spatial cooling. This binary molecular/noble gas approach provides a robust, low-loss route for spectral engineering in HCFs.

LaSo, UFS

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Optics Letters
51 (2026 17, 4813-4816

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Combined, table-top extreme-ultraviolet ellipsometry and polarimetry for studying ultrafast processes in matter

L. Gulyás Oldal, B. Gilicze, T. Bartyik, D. Kiss, M. Devetta, G. Zeni, F. Frasetto, L. Poletto, T. Csizmadia, and B. Major

We demonstrate the characterization of the complete polarization state of broadband extreme-ultraviolet radiation produced via high-harmonic generation in a gas target, measured with a double-stage polarimeter and a reaction microscope. The ellipsometric parameters of the reflective optics used in the polarimeter — meaning the extinction ratios and phase shift — were determined simultaneously. The results serve as a basis for table-top extreme-ultraviolet polarimetric and ellipsometric measurements, allowing ultrafast studies of polarization-sensitive matter, which require exact knowledge of the polarization state of the ionizing radiation.

LaSo, SeSo

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Journal of Physics: Photonics 8 (2026) 01LT01

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High-order exponential solver method for particle-in-cell simulations

Sz. Majorosi, N. A. M. Hafz, and Zs. Lécz

Outstanding advances in solid-state laser technology, employing the optical parametric chirped-pulse-amplification (OPCPA) technique, have led physicists to focus laser pulses to highly- relativistic intensities which led to novel schemes for charged-particle acceleration and radiation generation in laser-driven plasmas. Microscopic understanding of these highly-nonlinear processes is possible via accurate modeling of the laser-plasma interaction using particle-in-cell (PIC) simulations. Numerous codes are available and they rely on finite difference time domain methods on Yee-grids or on the analytical solution of the Maxwell-equations in spectral space. In this work, we present a solution bridging these two methods, which we call finite difference exponential time domain solution. This scalable method is able to provide very high accuracy even in 3D, but with improved locality, similar to the pseudospectral analytical methods without relying on transformation to special basis functions. We verified the accuracy and the convergence of the method in various benchmarks, including laser propagation in vacuum and in underdense plasma. We also simulated electron injection in a non-linear laser-plasma wakefield acceleration and surface high-harmonic generation in the overdense regime. The results are then compared with those obtained from standard PIC codes.

SeSo

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Computer Physics Communications 322 (2026) 110054

>>>

Bubble merging in laser wakefield acceleration as a way towards high-charge 1-GeV class electron beams

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Laser wakefield acceleration offers ultra-high accelerating gradients, enabling compact sources of multi-GeV electron beams with femtosecond durations and quasi-monoenergetic spectra. In this work, we investigated the nonlinear evolution of plasma bubbles and their effect on electron injection and energy gain, using high-fidelity, multi-dimensional particle-in-cell (PIC) simulations performed with the open-source code SMILEI. A relativistically intense laser pulse (a0=7.7, λ0=0.8 μm, w0=20 μm, E = 30 J, and τ=30 fs) propagated through a helium gaseous medium with a plateau density of ne =7 × 1018 cm-3 after complete ionization. The simulations revealed complex bubble dynamics, including initial formation, disruption, destruction, and bubble merging, strongly influenced by local longitudinal electric field Ex approaching or exceeding the cold wave-breaking limit EWB. Exceeding the wave-breaking field EWB triggered bubble destabilization, while the bubble merging at the end of the plateau plasma density region extended the acceleration length, sustaining high longitudinal fields on the order of 1 TV m-1 and boosting continuous electron injection. This mechanism produced a dense, quasi-monoenergetic electron bunch with a charge of 1 nC, a peak energy of ∼1 GeV, femtosecond-scale duration, energy spread below 10%, rms angular divergence of θy of 7 mrad, and a longitudinal rms beam size of σx=10 μm. Comprehensive analysis of the wakefield evolution demonstrated that exploiting nonlinear bubble evolution and interactions near the wave-breaking limit can enhance both energy gain and electron beam quality, providing actionable strategies for next-generation compact LPAs.

SeSo

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EPL 155 (2026) 24001

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Carbon ion acceleration in multi-component gas jets

Zs. Lécz, Sz. Majorosi, and Ch. Kamperidis

Laser-driven ion acceleration has been a central topic of the last two decades in the field of relativistic laser-plasma physics. As the target density shifts from overdense towards near-critical values, the complexity of the acceleration process increases, leading to the identification of new mechanisms and hybrid schemes. A change in targetry, from conventional solid or liquid jets, has been motivated by applications requiring high repetition rates, thus swiftly replenishable targets. Here, we computationally investigate the acceleration of carbon ions, highly relevant to radio-biology, and focus on the effect of the shape of a gas jet containing multiple ion species and on the effect of pulse duration. We show that smaller density gradients are suitable to reach 100 MeV/nucleon, with a required laser pulse duration ~100 fs and energy 200 J. We also demonstrate a piston-like effect of a higher-Z atom species (such as Ar) on the carbon ions.

SeSo

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EPL 155 (2026) 24001

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Single attosecond extreme ultraviolet pulse source via light-wave-controlled relativistic laser–plasma interaction: Thomson backscattering scheme

M. Shirozhan, F. Quéré, and S. Kahaly

Reflecting light off a mirror moving near light speed offers a powerful method for generating bright, ultrashort pulses in the extreme ultraviolet range. Several investigations show that dense relativistic electron mirrors can be created by striking a nanometer-scale foil with a high-intensity, sharp-fronted laser pulse, forming a single relativistic electron sheet (RES). This RES coherently reflects and upshifts a counterpropagating laser beam from the infrared to the extreme ultraviolet with efficiency exceeding incoherent scattering by over several orders of magnitude. Here, we demonstrate that optimizing the drive laser waveform can reliably produce a single RES, leading to the generation of isolated attosecond pulses enhancing both the intensity and temporal compression of the back-reflected light in a controlled manner. Simulations reveal that tuning parameters like timing delay enables control over the amplitude, duration, and bandwidth of the resulting attosecond Thomson backscattering pulse. Together, these advances meet key experimental challenges and pave the way for compact, tunable sources of isolated attosecond pulses for probing ultrafast phenomena.

SeSo

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Ultrafast Science
6 (2026) 0130

>>>

Impact ionization mediated terahertz nonlinearity of toroidal resonance

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Nonlinear and efficient control of terahertz (THz) waves is vital for advancing compact photonic technologies, including high-speed wireless communication, nonlinear optics, and tunable THz sources. However, realizing strong nonlinear responses even at moderate field strengths remains a significant challenge. In this work, we introduce a nonlinear, self-consistent THz modulation scheme based on a dual toroidal metasurface fabricated on high-resistivity silicon. When excited by sub-picosecond THz pulses with peak electric fields ranging from 90 to 450 kV cm–1, the metasurface induced strong field-confinement facilitates impact ionization, resulting in a carrier density increase from $\approx 10^{10}$ cm^{-3} to 2.9×10^{18} cm^{-3} and a corresponding conductivity enhancement from $\approx 1 \times 10^{-12}$ to 5806 S m^{-1}. These THz-driven changes, as revealed by a theoretical analysis, lead to a complete suppression of both toroidal and LC resonances, and a strong nonlinear behavior. Further the scattering power drops by more than two orders of magnitude near THz probe strength of 300 kV cm^{-1}; close to the avalanche breakdown threshold of silicon, hence confirming impact ionization driven self-consistently tunable toroidal resonances. These findings underscore the effectiveness of nonlinear THz modulation for integration into next-generation compact silicon photonic platforms while opening up new avenues in THz research. More importantly, we demonstrate that mode engineering provides an additional and powerful pathway to enhance device performance beyond conventional resonance-based designs.

SeSo

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Advanced Optical Materials
14 (2026) 25, e71367

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Broadband GaP contact-grating terahertz source pumped at 3.9 μm

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A gallium phosphide (GaP) semiconductor contact-grating THz source with trapezoidal grating groove profile, pumped at a mid-infrared wavelength of 3.9 μm, was demonstrated. The source can be scaled to high electric fields beyond 1 MV/cm due to the plane-parallel geometry, the availability of large GaP single crystals of good quality, and the large bandwidth extending from 0.2 THz to 6 THz. Due to the long pump wavelength, the lowest-order effective multiphoton absorption was 9-photon absorption, which enabled exceptionally high usable pump intensities up to 310 GW/cm^2. Saturation of THz generation efficiency occurred at a high pump intensity of about 160 GW/cm^2, caused by pump-induced free-carrier generation which can be explained by multiphoton and Keldysh tunnel ionization models.

SeSo

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Optics Express
34 (2026) 8, 13663

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Propagation effects in high harmonic generation media driven by bright squeezed vacuum light

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Recent developments in quantum light engineering have enabled the use of infrared bright squeezed vacuum (BSV) femtosecond pulses in nonlinear optics, including strong-field physics and high-harmonic generation. However, theory has focused on single-atom interactions, neglecting the crucial macroscopic aspect of light propagation through media. This raises a key question: How does BSV propagate in nonlinear media, and how this affects the nonlinear signals and the radiation's quantumness? We address this with a fully quantized framework for propagation in gas media undergoing high-harmonic generation. We find that ionization and the associated photon losses cause decoherence, which limits the propagation length, degrades radiation's quantumness, and reduces the emitted harmonics. However, these effects are not detrimental. We identify conditions that minimize propagation-induced decoherence while preserving detectable harmonics with super-Poissonian photon statistics. Our results establish fully quantized basis for exploring BSV in nonlinear optics, strong-field-quantum optics, and ultrafast science in all states of matter.

SeSo

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Nature Communications
17 (2026) 8457

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Monitoring gold nanoparticle formation by in situ transient absorption spectroscopy

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Performing ultrafast spectroscopy during nanoparticle synthesis can provide new insights into the kinetics and mechanism of nanoparticle formation. In these experiments, we thoroughly studied the ultrafast decay of the transient absorption signal from reference gold nanoparticles (with well-defined diameters of 5, 20, and 40 nm) and from synthesized gold nanoparticles with 1:1 and 1:4 gold-to-citrate molar ratio. The application of the high repetition rate laser (100 kHz) with short pump pulse duration (10 fs, 470–570 nm) allows the rapid in situ TAS monitoring of the particle growth. Following excitation with femtosecond pulses, the acoustic vibrations of the particles produced periodic oscillations in the transient absorption signal. The decay traces at the selected wavelengths were fitted, and the Fast Fourier Transform (FFT) analysis was used for the determination of the characteristic frequencies of the acoustic vibrations. The frequency of the periodic oscillations decreases with an increasing size. We demonstrate that the formation of monodisperse gold nanoparticles at 75 °C can be monitored during the synthesis, providing direct evidence about their quality and particle size in the 12–55 nm particle diameter range. We concluded that the average primary size of the monodisperse gold nanoparticles increased in the 19–23 min synthesis time range as the frequency of the acoustic vibrations decreased for the Au-Cit 1:4 sample and remained constant in the last phase of the synthesis.

LaSo, UFS

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Journal of Physical Chemistry C
130 (2026) 3, 1225-1235

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Machining of Fe-based amorphous alloy ribbons with sub-50 femtosecond laser pulses

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Fe-based metallic glasses are ideal candidates to be utilized in transformer cores owing to their outstanding soft magnetic properties. However, they are difficult to machine properly by conventional means due to their mechanical brittleness and poor thermal conductivity. Here, the cutting of Fe_{91}-$Si_{4.5}$-$C_{4.0}$-$Al_{0.5}$ amorphous alloy ribbons is reported with a sub-50 fs laser pulses. A systematic study is performed on local morphological and chemical composition changes to the machined edge in comparison to crystalline metals. It is shown that only the innermost 80 µm wide region of the cut edge shows any detectable modifications, which is much less than for continuous laser machining. Therefore, the proposed method is indeed a valuable approach to overcome the fine machining difficulties of metallic glasses.

LaSo, UFS, Eng

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Micromachines
17 (2026) 2, 214

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Gold nanoparticle-embedded cellulose acetate: structural, optical, mechanical, and cytotoxicity assessment

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The development of composites with embedded gold nanoparticles (Au NPs) and biopolymeric matrices, such as cellulose acetate (CA), has gained significant attention due to their unique synergistic properties, including enhanced mechanical, physical, and thermal characteristics. In this study, a composite material consisting of Au NPs embedded in a CA matrix was prepared and thoroughly characterized and its cytotoxicity evaluated for potential medical applications such as drug delivery, biosensing, and imaging. The composite was prepared using a newly developed in situ method, ensuring mostly uniform dispersion of Au NPs within the CA matrix. Various characterization techniques, including X-ray diffraction (XRD), scanning electron microscopy (SEM), atomic force microscopy (AFM), energy-dispersive X-ray spectroscopy (EDX), X-ray photoelectron spectroscopy (XPS), UV-Vis spectroscopy, Fourier transform infrared spectroscopy (FTIR), dynamic mechanical analyses (DMA), thermogravimetric analysis (TGA), and cell viability assay were employed to evaluate the structural, mechanical, thermal and biocompatibility properties of the as-prepared composite. The obtained results indicate that even a miniscule content of Au NPs (<0.14 wt%) within the CA matrix can significantly change the properties of such composites. The produced materials are compact, flexible, strong, and exhibit low cytotoxicity, making them suitable for a wide range of potential applications.

UFS

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Materials Advances
7 (2026) 798-812

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Ultrafast electron intervalley scattering and hole dynamics in amorphous and crystalline Ge

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The development of composites with embedded gold nanoparticles (Au NPs) and biopolymeric matrices, such as cellulose acetate (CA), has gained significant attention due to their unique synergistic properties, including enhanced mechanical, physical, and thermal characteristics. In this study, a composite material consisting of Au NPs embedded in a CA matrix was prepared and thoroughly characterized and its cytotoxicity evaluated for potential medical applications such as drug delivery, biosensing, and imaging. The composite was prepared using a newly developed in situ method, ensuring mostly uniform dispersion of Au NPs within the CA matrix. Various characterization techniques, including X-ray diffraction (XRD), scanning electron microscopy (SEM), atomic force microscopy (AFM), energy-dispersive X-ray spectroscopy (EDX), X-ray photoelectron spectroscopy (XPS), UV-Vis spectroscopy, Fourier transform infrared spectroscopy (FTIR), dynamic mechanical analyses (DMA), thermogravimetric analysis (TGA), and cell viability assay were employed to evaluate the structural, mechanical, thermal and biocompatibility properties of the as-prepared composite. The obtained results indicate that even a miniscule content of Au NPs (<0.14 wt%) within the CA matrix can significantly change the properties of such composites. The produced materials are compact, flexible, strong, and exhibit low cytotoxicity, making them suitable for a wide range of potential applications.

UFS

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Physical Review B
113 (2026) 205204

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Multimodal radiosensitization by hafnium oxide nanoparticles and HDAC inhibitors: mechanistic insights

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Radiation therapy is routinely utilized in cancer treatment, often in combination with chemotherapy, but is limited by collateral damage to healthy tissues and radioresistance of some tumors Radiosensitizing agents can enhance tumor cell susceptibility to ionizing radiation, allowing effective treatment at lower doses. High-atomic-number metal-based nanoparticles, such as hafnium oxide (HfO_2NP), can locally amplify the impact of ionizing radiation on cancer cells, augment the radiation-triggered generation of reactive electrons and oxygen species (ROS), induce DNA damage, and ultimately lead to cell death. We hypothesized that this effect can be further enhanced by histone deacetylase (HDAC) inhibitors, which maintain the chromatin in a relaxed state and render the DNA more accessible to genotoxic stress. In this study, we found that HfO_2NPs and the HDAC inhibitor, when combined with irradiation, induced significantly higher ROS production, massively reduced mitochondrial membrane potential, and increased DNA double-strand break formation in cancer cells compared to untreated or single-agent-treated cells. These effects led to a marked reduction in colony-forming potential in both 2D and 3D models and induced significant apoptosis. No cytotoxicity was observed in non-cancerous fibroblasts. HfO_2NPs and the tested HDAC inhibitor form a remarkably efficient cancer-selective radiosensitizing combination, where the enzyme inhibitor facilitates the irradiation-induced DNA-damaging potential of the nanoparticles. This outstanding multimodal approach can target radioresistant cancer cells, while not affecting healthy cells, underscoring its potential in a next-generation nanomedicine-based radiosensitizing strategy to attenuate cancer cell growth for an improved therapeutic outcome.

UFS

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Nanoscale Advances
8 (202) 2003-2020

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Structural reorganization drives exciton relaxation pathways in layered 2D Ruddlesden–Popper (RP) perovskite BA_2PbI_4

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2D halide perovskites are promising materials for optoelectronics due to their strong excitonic effects and soft, dynamically active lattices. Synthesis conditions, particularly thermal annealing, play a critical role in tuning their structural and excitonic properties by influencing lattice vibrations and defect states. The impact of structural reorganization in 2D Ruddlesden–Popper (RP) n-butyl ammonium lead iodide (BA_2PbI_4) has been systematically characterized using various state-of-the-art experimental techniques, such as temperature-dependent X-ray diffraction (XRD), temperature-dependent photoluminescence (TDPL), temperature-dependent resonance Raman spectroscopy, terahertz time-domain spectroscopy (THz-TDS), transient absorption spectroscopy (TAS), and further supported by first-principles DFT calculations, reveals a direct link between thermal processing and structural dynamics. Raman spectra show broadened low-frequency modes in the annealed sample, indicative of enhanced lattice anharmonicity. THz-TDS reveals stronger phonon absorption near 2 THz, aligning with Raman-active modes and confirming increased lattice anharmonicity. The 2 THz phonon mode in the annealed film exhibits a nearly threefold increase in oscillator strength (OS), calculated by integrating the real part of the optical conductivity between 0.2 and 2.5 THz, increasing from 39.01 S m^{-1} THz in the as-grown film to 146.19 S m^{-1} THz after annealing, indicating enhanced exciton–phonon coupling; this is further complemented by TDPL measurements, which show more pronounced self-trapped exciton (STE) emission in the annealed film below ~270 K, collectively corroborating strong exciton–phonon coupling. Transient absorption spectroscopy shows longer carrier lifetimes (~1.7 ns) in the annealed film vs. the as-grown (~1.1 ns), consistent with increased exciton localization. Thermal annealing boosts lattice dynamics and exciton–phonon coupling, offering a strategy for future low-dimension material design.

UFS

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Small
22 (2026) 31, e09142

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Tuning the optoelectronic and photovoltaic properties of natural chlorophyll dye molecules via solvent interaction: A computational insight

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The chlorophyll molecule is considered a low-cost material, easy to synthesize, and easily extracted from plant leaves. It exhibits high chemical stability, structural flexibility, and high absorbance ability at the visible range of electromagnetic radiation. In this work, the geometrical, electronic, and optical properties of pure, dissolved, and doped chlorophyll (C1) natural organic dye were computed by density functional theory (DFT) and time-dependent density functional theory (TD-DFT). The solvents considered include water (H_2O), acetone (C_2H_6O), dichloromethane (CH_2Cl_2), chloroform (CH_3Cl), and dimethyl-sulfoxide (DMSO) (C_2H_6OS). The solar photovoltaic parameters, such as light-harvesting efficiency (LHE), oscillation strength (f), free energy of electron injection (ΔGInj.) and regeneration (ΔGReg.), open-circuit voltaic (VOC), and efficiency (η), were also investigated. The evaluated energy gap slightly shifted from 1.920 eV to 1.980 eV based on the solvent polarity, while the UV-Visible absorption spectrum red-shifted from 422.3 nm to 439.8 nm, improving the overall efficiency up to 21.5% in DMSO solvent. The (LHE) and (ΔGInj.) properties regarding Cl molecules improved up to 69.1% and –1.384 eV when dissolved in chloroform and DMSO solvents, respectively. Doping C1 molecule via metal transition atoms such as zinc (Zn), nickel (Ni) and copper (Cu) further modified the optical and photovoltaic performance. Doped C1 molecule via Cu atom shows the best photonic results, including the highest open-circuit voltage (Voc) and conversion efficiency (η), while the Ni-doped C1 dye displays the longest lifetime, 1.699 μs, and the highest electronic coupling constant, 1.975 eV; thus, it has the superior photovoltaic performance. These results demonstrate that both solvents and transition metal atom modification significantly improve C1 performance, making metal-doped C1 a promising low-cost and eco-friendly sensitizer for dye-sensitized solar cells (DSSCs).

UFS

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Nanomaterials
16 (2026) 6, 365

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The synthesis of boron-, carbon-, and nitrogen-containing 2D materials on Ir(111): Tthe role of boron carbide

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The preparation of mixed boron-, carbon-, and nitrogen-containing 2D materials has been intensively studied to optimize their electronic properties. For this purpose, the decomposition of bis-BN cyclohexane ($B_2N_2C_2H_{12}$) was studied in this work on Ir(111) using electron diffraction as well as core and valence band photoemission. The underlying energetics has been disclosed by density functional theory calculations. The expectation that a precursor with all three elements in its ring would facilitate the formation of atomically mixed BCN films was not met. When the molecules were adsorbed at 50 °C, followed by subsequent annealing, the rupture of the six-membered rings started already at 275 °C. The preparation of the overlayer in the range of 650 °C – 740 °C primarily resulted in the formation of phase-separated h-BN and graphene domains. However, increasing the preparation temperature to 980 °C – 1110 °C considerably enhanced mixing. At the obtained N-deficient average compositions: (i) the average size of h-BN islands decreased much, down to ~1 nm or below, and they were mostly terminated by B atoms; (ii) the area covered by extended h-BN domains decreased and disappeared; (iii) surplus B atoms were alloyed into graphene forming a 2D boron carbide matrix in which h-BN nanodomains are embedded; (iv) the edge region of h-BN nanoislands can be considered chemically a one-dimensional mixed BCN phase. Our results revealed that the presence of boron carbides should also be considered when studying BCN layers. For the first time, we experimentally characterized their band structure by momentum microscopy.

UFS

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Carbon
256 (2026) 121783

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Design strategy for influencing hot carrier cooling dynamics in low-dimensional perovskites

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The structural landscape of low-dimensional perovskites, modulated by the organic spacer cation, governs the relaxation of hot carriers. Using transient absorption spectroscopy and molecular dynamics simulations, we show that spacer-induced octahedral distortions and lattice rigidity define the balance between polaronic screening and phonon-driven relaxation. We found that the phenethylammonium spacer induces significant distortions and stronger exciton-phonon coupling, favoring polaron formation and delayed carrier cooling. In contrast, a rigid bithiophenethylammonium spacer suppresses distortions, stabilizes coherent phonons, and accelerates thermalization, while thiopheneethylammonium represents intermediate behavior. The structure-phonon-carrier interplay reconciles conflicting views on hot-carrier dynamics, revealing that soft lattices stabilize polarons, whereas rigid heteroatom-containing conjugated spacers activate efficient phonon relaxation pathways. This structural picture operates alongside a coupled electronic contribution from spacer-derived electronic states within the conduction manifold, which provides an additional relaxation pathway, indicating that lattice rigidity and electronic coupling are intrinsically coupled rather than acting independently. These insights provide molecular design principles for tailoring carrier relaxation, guiding perovskite engineering toward optoelectronic devices and the efficient harnessing of hot carriers.

UFS

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Advanced Energy Materials

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Wave packet motion in a quantized electromagnetic field: analytic results

Sz. Hack, B. G. Pusztai, K. Joós, S. Varró, A. Czirják, and P. Földi

We investigate the dynamics of a charged particle interacting with a multimode quantized electromagnetic field and obtain an analytic solution for the full electron-field system. In the present finite-mode formulation the total electron-field dynamics remains closed and unitary. The framework enables the calculation of position expectation values and uncertainties for arbitrary wave packets and field states, allowing us to identify quantum corrections to the corresponding classical motion. While the corrections to the position expectation value are weak and largely insensitive to the quantum state of the field, the wave packet broadening exhibits a pronounced dependence on the field state. In particular, the quantum uncertainty of the radiation is directly imprinted onto the spatial uncertainty of the particle. We illustrate these effects for Gaussian wave packets interacting with coherent, Fock, and squeezed states, including bright squeezed vacuum. The interaction with a finite-duration laser pulse is also analyzed as a multimode example. Our results provide a transparent analytic route toward understanding how quantum fluctuations of light influence electron dynamics in strong-field settings.

UFS

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New Journal of Physics
28 (2026) 074510

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Low-energy proton impact dynamics on hydrocarbons: Dependence on kinetic energy and incident site

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The dynamics of low-energy proton collisions with hydrocarbon molecules are investigated using real-time time-dependent density functional theory. Through systematic variation of proton kinetic energy and impact site on the molecular surface, the resulting scattering, proton capture, and bond dissociation pathways are analyzed. The simulations reveal a strong dependence of reaction outcomes on both incident energy and collision geometry, with the interplay between electronic and nuclear degrees of freedom highlighted as governing molecular fragmentation and reaction mechanisms. These findings provide insight into the fundamental processes underlying proton–hydrocarbon interactions relevant to radiation chemistry, ion-beam processing, astrochemical environments, and Coulomb explosion.

UFS

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AIP Advances
16 (2026) 045318

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Chirp- and CEP-dependence of HHG spectra simulated by an upgraded one-dimensional atomic model potential

K. Sallai, Sz. Hack, Sz. Majorosi, P. Földi and A. Czirják

We investigate the accuracy of a recently introduced upgraded one-dimensional (1D) atomic model potential, the Gaussian windowed soft-core Coulomb (GSC) potential, in typical strong-field physics scenarios. In particular, we consider linearly polarized near-infrared femtosecond laser pulses with different carrier-envelope phase (CEP) and chirp values. By comparing the results of 1D and three-dimensional simulations, we show that the GSC potential reproduces the effects of CEP and chirp on the high-order harmonic generation spectra with good overall accuracy for both the spectral amplitude and phase, including also subtle features like a double-plateau in certain cases.

UFS

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Physica Scripta
101 (2026) 35, 355406

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Photoelectron holography in a pump-drive setup

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We have investigated theoretically the formation of photoelectron holograms in the momentum distribution of the continuum electrons generated during the ionization of H atoms by ultrashort laser pulses. In previous theoretical and experimental works the observation of a clear holographic interference pattern was hindered by other secondary processes like the temporal interference or the presence of electron trajectories with multiple scattering events. In the present work we present a two-pulse setup for the production of clear photoelectron holograms. In this pump-drive setup an attosecond laser pulse is used for the creation of the continuum wave packet, while a second longer laser pulse is used to drive the dynamics of the continuum wave packet. By performing calculations for different pump-drive delays for a given drive-pulse shape, we have identified the optimal delay value for the production of the photoelectron holograms. We also verified for this optimal delay value how the photoelectron hologram can be shaped by varying the wavelength and intensity of the drive pulse.

UFS

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Physical Review A
113 (2026) 1, 013107

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Light-induced nonadiabatic photodissociation of the NaH molecule including electron-rotation coupling

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It is well established that electronic conical intersections (CIs) in molecular systems can be induced by laser light, even in diatomic molecules. The emergence of these light-induced degeneracies leads to strong coupling among electronic, vibrational, and photonic modes, which significantly influences ultrafast nuclear dynamics. In this work, we perform pump-probe numerical simulations on the NaH molecule, considering the first three singlet electronic states [$X^1\sum+(X)$, $A^1\sum+(A)$, and $B^1\prod(B)$] and including several light-induced degeneracies in the theoretical model. To elucidate the ultrafast molecular dynamics, we study the combined effects of multiple light-induced nonadiabatic couplings and rotational motion of the nuclei together with the situation when the electronic angular momentum projected onto the diatomic axis couples with the angular momentum of the nuclei. We then calculate key dynamical observables such as dissociation probabilities, kinetic energy release (KER) spectra, and angular distributions of the photofragments within and above the linear regime. The discrepancies between the different employed models are relatively minor for the dissociation probabilities and KER spectra. In contrast, for angular distributions, the inclusion of electronic spin and orbital angular momentum leads to substantial differences between the three applied schemes in the small ejection angle region.

UFS

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Physical Review
A 113 (2026) 5, 052815

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Light-induced nonadiabatic dissipative quantum dynamics of the Na_2 molecule

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Strong light–matter coupling between molecules and optical or plasmonic cavity modes has emerged as a promising platform for advancing photonics, materials science, and chemistry. However, optical cavities and plasmonic resonators in particular are inherently lossy systems characterized by finite photon lifetimes. Accurate theoretical descriptions of molecular dynamics under strong coupling therefore require a proper treatment of cavity losses. In this work, we compare three theoretical approaches for modeling dissipative molecule–cavity dynamics within a realistic parameter regime: the Lindblad master equation, the stochastic Schrödinger equation, and the non-Hermitian Schrödinger equation. As an example, we consider the two lowest electronic energy states of the Na_2 molecule coupled to a cavity mode and analyze the time evolution of the excited-state population and the mean photon number. Our results demonstrate that the stochastic Schrödinger equation provides an accurate and computationally efficient alternative to the Lindblad master equation, while the non-Hermitian Schrödinger approach is found to be applicable only within a limited range of conditions. Furthermore, we show that inclusion of molecular rotation leads to rotational–vibrational–photonic coupling and gives rise to pronounced nonadiabatic dynamics through light-induced conical intersections. These findings highlight the importance of both dissipation and rotational degrees of freedom for a realistic description of molecular dynamics in strongly coupled molecule–cavity systems.

UFS

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J. Chem. Phys.
165 (2026) 094303

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Large area materials processing via unfocused beams of high-energy femtosecond lasers

J. Bohus, Á. Mohácsi, A. P. Farkas, L. Égerházi, B. Hopp, and T. Szörényi

Petawatt-class laser systems can generate intensities sufficient for material processing even without beam focusing. However, their inhomogeneous energy distribution renders them unsuitable for producing macroscopically uniform patterns. In this study, this limitation is turned into an advantage: upon irradiation with the entire beam cross-section, the surface encodes the spatial energy distribution as a material response library, enabling systematic analysis based on the robust dataset obtained. This framework provides a single-step methodology for determining optical and morphological thresholds, offering an alternative to conventional Laser-Induced Damage Threshold (LIDT) protocols.

As a proof of concept, copper was irradiated by a stationary beam from a diode-pumped ytterbium femtosecond laser (500 mJ and 500 fs at 1030 nm/50 Hz). A reflectance map obtained using a He–Ne probe was correlated with the energy distribution of the processing beam. The morphological processes behind the energy-dependent darkening were examined through constructing a surface morphology map from scanning electron microscopy (SEM) images taken at 5,000–50,000 × magnifications. The reflectance-based darkening threshold energy, marking the first visible modification, was 1.46 μJ (≈0.023 J·cm^{-2} in terms of fluence), while the morphological threshold appeared at 1.2 μJ, indicating the onset of nanostructure formation. Maximum darkening occurred between 2.4–2.6 μJ, associated with a hierarchical morphology of cauliflower-like microtexture and a highly homogeneous nanostructure, followed by reflectance recovery above 2.8 μJ due to melting and coalescence. Gray-Level Co-Occurrence Matrix (GLCM) texture analysis revealed that homogeneity sensitively indicated the onset of ablation, whereas contrast and entropy reflected changes in granularity and structural order.

LaSo, Eng

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Applied Surface Science 727 (2026) 165974

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Surface nanoprocessing with unfocused beams of high-energy femtosecond lasers: A tool to produce surface characteristics libraries

J. Bohus, Á. Mohácsi, A. P. Farkas, L. Égerházi, and T. Szörényi

We demonstrate a single-shot method for probing ultrafast laser–matter interactions using unfocused multi-terawatt femtosecond beams. The intrinsic fluence inhomogeneity of the beams is exploited to accomplish parallel, spatially encoded experiments performed under strictly identical conditions across a wide energy range in a single step, enabling systematic mapping of energy-dependent surface responses without beam scanning. As proof of the technique, the large set of simultaneously collected data points below, at, and above the threshold inherently allows for a threshold evaluation approach, different from both the diameter/depth regression analysis and the statistical method. Using copper as a test system, we quantify the fluence dependence of reflectance and morphology and identify a multi-pulse optical threshold of 0.020 J/cm^2, coinciding with the onset of ablation confirmed by SEM imaging. The minimum specular reflectance observed, around 0.10%, favorably compares to the respective figures reported. Applying this parallelized surface mapping technique with high-energy laser systems featuring suitably large beam diameters thereby provides a versatile platform for exploring ultrafast laser-induced surface responses, with potential applications in material design, surface engineering, and optical damage studies.

LaSo, Eng

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Applied Physics Letters
128 (2026) 101906

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Asymmetric self-injection of electrons in a laser wakefield accelerator via localized laser redshifting

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Propagation of intense laser pulses in underdense plasma always involves nonlinear evolution of the laser envelope, which leads to large deviations from the initial Gaussian intensity profile. The modulations in the intensity envelope have strong influence not only on the formation of the wakefield, but also in the process of electron injection; thus, it defines the final spectral and angular distribution of the accelerated electrons. Better understanding of the laser pulse evolution is crucial for the correct interpretation of the experimental results, especially in the highly relativistic regime. We developed a simple numerical tool, which adequately models the evolution of the laser envelope up to the point when the spectral broadening becomes significant. Our numerical modeling sheds light on the asymmetric wakefield generation and consequent off-axis injection of electrons, observed in experiments and particle-in-cell simulations.

LaSo, SeSo, Eng

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Physical Review Research
8 (2026) 023080

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Development of micro-CT-based anatomically accurate tooth model for finite element analysis of composite restorations

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Background: Finite element analysis (FEA) has become an important tool in restorative dentistry for investigating stress distribution in teeth and dental restorations. However, the accuracy of such analyses strongly depends on the anatomical fidelity of the underlying tooth models, which is often limited in simplified geometries. The objective of this study was to develop an anatomically accurate three-dimensional tooth model based on micro-computed tomography (micro-CT) data and to evaluate the biomechanical behaviour of sound and composite-restored teeth under clinically relevant loading conditions.

Methods: A human tooth was scanned using high-resolution micro-CT imaging. Enamel, dentin, and pulp were segmented and reconstructed into three-dimensional geometries, which were further refined using computer-aided design (CAD) tools. The resulting models were imported into a finite element environment for mechanical simulation. Static loading conditions were applied to both sound and composite-restored tooth models, including a vertical load of 200 N and an oblique load of 200 N applied at a 45° angle to the tooth crown. Von Mises stress distributions were evaluated to characterize stress concentration patterns.

Results: Finite element simulations revealed maximum von Mises stresses of approximately 140 MPa, predominantly localized in the coronal regions of the tooth. Oblique loading produced increased and more asymmetric stress concentrations than vertical loading, particularly in the anterior and posterior crown regions. While overall stress distributions were comparable between sound and composite-restored teeth, locally increased stress levels were observed in restored models under oblique loading. Conclusions: Anatomically accurate, micro-CT-based finite element tooth models provide a robust framework for biomechanical analysis in restorative dentistry. The presented workflow enables detailed evaluation of stress distribution in composite-restored teeth and may contribute to improved understanding and optimization of restorative materials and treatment strategies.

Eng

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Dentistry Journal
14 (2026) 5, 279

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