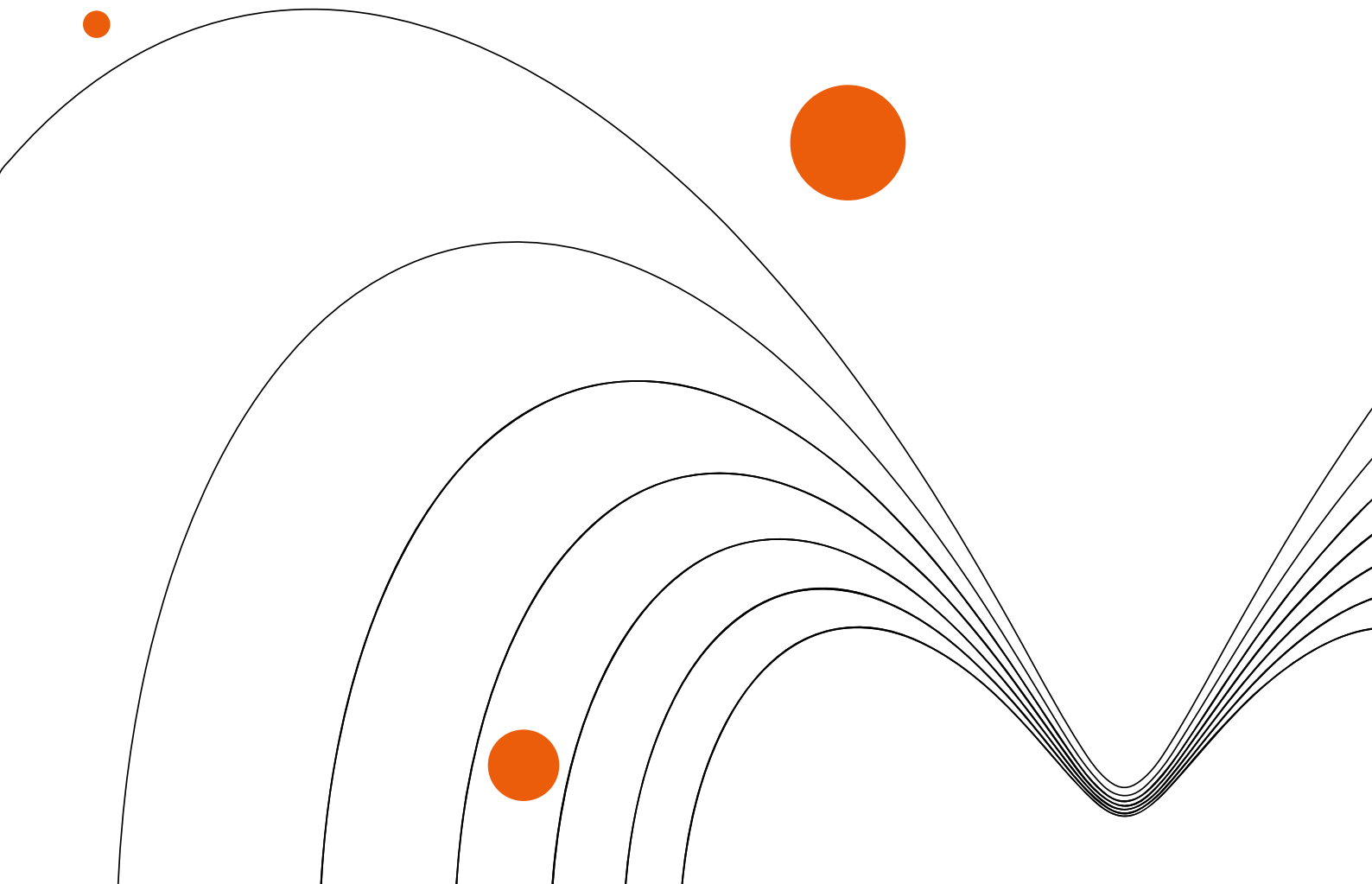


# ABSTRACTS

ELI ALPS | 2024





# Systematic comparison of commercial devices for temporal characterization of few-cycle laser pulses in the 500-1000 nm spectral range

● V. Pajer, J. Bohus, A. Malakzadeh, L. Lehotai, M. Kalashnikov, I. Seres, B. Gilicze, B. Kiss, Á. Börzsönyi, K. Varjú, G. Szabó, and R. Nagymihály

We compare multiple temporal pulse characterization techniques in three different pulse duration regimes from 15 fs to sub-5 fs, as there are no available standards yet for measuring such ultrashort pulses. To accomplish this, a versatile post-compression platform was developed, where the 100 fs near infrared pulses were post-compressed to the sub-two-cycle regime in a hybrid, three-stage configuration. After each stage, the duration of the compressed pulse was measured with the d-scan, TIPTOE and SRSI techniques and the retrieved temporal intensity profiles, spectrum and spectral phases were compared. Spectral homogeneity was also measured with an imaging spectrometer to understand the input coupling conditions of the temporal measurements. Our findings suggest that the different devices give similar results in terms of temporal intensity profile, however they are extremely sensitive to alignment and to beam quality, especially in the case of the shortest pulses. We address specific steps of measurement procedures, which paves the way towards the standardization of pulse characterization in the near future.

## LaSo

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**Optics Express**  
**32 (2024) 9 15710-15722**





# Quantum-optical analysis of high-order harmonic generation in $H_2^+$ molecules

● J. Rivera-Dean, P. Stammer, A. S. Maxwell, Th. Lamprou, E. Pisanty, P. Tzallas, M. Lewenstein, and M. F. Ciappina

We present a comprehensive theoretical investigation of high-order harmonic generation in  $H_2^+$  molecules within a quantum-optical framework. Our study focuses on characterizing various quantum-optical and quantum-information measures stemming from the correlations established between light and matter. We demonstrate the emergence of entanglement between electron and light states after the laser-matter interaction. We also identify the possibility of obtaining nonclassical states of light in targeted frequency modes by conditioning on specific electronic quantum states, which turn out to be crucial in the generation of highly nonclassical entangled states between distinct sets of harmonic modes. Our findings open up avenues for studying strong-laser-field-driven interactions in molecular systems under a fully quantum-mechanical framework.

SeSo

Paraskevas TZALLAS

Physical Review A  
109 (2024) 033706





# Nonclassical states of light after high-harmonic generation in semiconductors: A Bloch-based perspective

● J. Rivera-Dean, P. Stammer, A. S. Maxwell, Th. Lamprou, A. F. Ordóñez, E. Pisanty, P. Tzallas, M. Lewenstein, and M. F. Ciappina

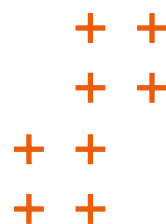
High-harmonic generation (HHG) has emerged as a pivotal process in strong-field physics, yielding extreme ultraviolet radiation and attosecond pulses for a wide range of applications. Furthermore, its emergent connection with the field of quantum optics has revealed its potential for generating nonclassical states of light. Here, we investigate the process of high-harmonic generation in semiconductors under a quantum optical perspective while using a Bloch-based solid-state description. Through the implementation of quantum operations based on the measurement of high-order harmonics, we demonstrate the generation of nonclassical light states similar to those found when driving atomic systems. These states are characterized using diverse quantum optical observables and quantum information measures, showing the influence of electron dynamics on their properties. Additionally, we analyze the dependence of their features on solid characteristics such as the dephasing time and crystal orientation, while also assessing their sensitivity to changes in driving field strength. This paper provides insights into HHG in semiconductors and its potential for generating nonclassical light sources.

SeSo

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Physical Review B  
109 (2024) 035203





# Wave packet dynamics and control in excited states of molecular nitrogen

- M. Fushitani, H. Fujise, A. Hishikawa, D. You, S. Saito, Y. Luo, K. Ueda, H. Ibrahim, F. Légaré, S. T. Pratt, P. Eng-Johnsson, J. Mauritsson, A. Olofsson, J. Peschel, E. R. Simpson, P. A. Carpeggiani, D. Ertel, P. K. Maroju, M. Moioli, G. Sansone, R. Shah, T. Csizmadia, M. Dumergue, H. N. Gopalakrishna, S. Kühn, C. Callegari, M. Danailov, A. Demidovich, L. Raimondi, M. Zangrando, G. De Ninno, M. Di Fraia, L. Giannessi, O. Plekan, P. Rebernik Ribic, and K. C. Prince

Wave packet interferometry with vacuum ultraviolet light has been used to probe a complex region of the electronic spectrum of molecular nitrogen,  $N_2$ . Wave packets of Rydberg and valence states were excited by using double pulses of vacuum ultraviolet (VUV), free-electron-laser (FEL) light. These wave packets were composed of contributions from multiple electronic states with a moderate principal quantum number ( $n \sim 4-9$ ) and a range of vibrational and rotational quantum numbers. The phase relationship of the two FEL pulses varied in time, but as demonstrated previously, a shot-by-shot analysis allows the spectra to be sorted according to the phase between the two pulses. The wave packets were probed by angle-resolved photoionization using an infrared pulse with a variable delay after the pair of excitation pulses. The photoelectron branching fractions and angular distributions display oscillations that depend on both the time delays and the relative phases of the VUV pulses. The combination of frequency, time delay, and phase selection provides significant control over the ionization process and ultimately improves the ability to analyze and assign complex molecular spectra.

SeSo

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**Harshitha N. GOPALAKRISHNA**  
**Sergei KÜHN**

**J. Chem. Phys.**  
**160 (2024) 104203**





# Novel spectrometer designs for laser-driven ion acceleration

● A. Morabito, K. Nelissen, M. Migliorati, and S. Ter-Avetisyan

We propose novel spectrometer designs that aim to enhance the measured spectral range of ions on a finite-sized detector. In contrast to the traditional devices that use a uniform magnetic field, in which the deflection of particles increases inversely proportional to their momentum, in a gradient magnetic field, the deflection of particles will decrease due to the reduction of the magnetic field along their propagation. In this way, low-energy ions can reach the detector because they are deflected less, compared to the uniform field case. By utilizing a gradient magnetic field, the non-linear dispersion of ions in a homogeneous magnetic field approaches nearly linear dispersion behavior. Nonetheless, the dispersion of low-energy ions, using a dipole field, remains unnecessarily high. In this article, we discuss the employed methodology and present simulation results of the spectrometer with an extended ion spectral range, focusing on the minimum detectable energy (energy dynamic range) and energy resolution.

SeSo

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Photonics  
11 (2024) 7, 605





# Tunable ultrafast thermionic emission from femtosecond-laser hot spot on a metal surface by control of laser polarization and angle of incidence: A numerical investigation

● M. Upadhyay Kahaly, S. Madas, B. Mesits, and S. Kahaly

Ultrafast laser induced thermionic emission from metal surfaces has several applications. Here, we investigate the role of laser polarization and angle of incidence on the ultrafast thermionic emission process from laser driven gold coated glass surface. The spatio-temporal evolution of electron and lattice temperatures are obtained using an improved three-dimensional (3D) two-temperature model (TTM) which takes into account the 3D laser pulse profile focused obliquely onto the surface. The associated thermionic emission features are described through the modified Richardson-Dushman equation, including dynamic space-charge effects and are included self-consistently in our numerical approach. We show that temperature-dependent reflectivity influences laser energy absorption. The resulting peak electron temperature on the metal surface monotonically increases with the angle of incidence for the P polarization, while for the S polarization it shows the opposite trend. We observe that thermionic emission duration shows a strong dependence on the angle of incidence and contrasting polarization dependent behavior. The duration of the thermionic current shows strong correlation to the intrinsic electron-lattice thermalization time, in a fluence regime well below the damage threshold of gold. The observations and insights have important consequences in designing ultrafast thermionic emitters using a metal based architecture.

**Seso, UFS**

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Saibabu MADAS  
Subhendu KAHALY**

**Applied Surface Science  
643 (2024) 158668**





# Atomic ordered doping leads to enhanced sensitivity of phosgene gas detection in graphene nanoribbon: a quantum DFT approach

● R. Deji, G. N. Nagy, B. C. Choudhary, R. K. Sharma, M. K. Kashyap, and M. Upadhyay Kahaly

We explore a novel sensor for detection of phosgene gas by graphene derivatives such as pristine and doped graphene nanoribbons via first principles calculations. The interaction of phosgene molecule with various edge and center doped configurations of boron, phosphorus and boron-phosphorus co-doped armchair graphene nanoribbon (AGNR) and zigzag graphene nanoribbon (ZGNR) is investigated through density functional theory (DFT). P-doped systems showcase chemisorption, displaying enhanced sensitivity to phosgene detection as reflected by a more negative adsorption energy values, accompanied by a prominent charge transfer due to the doping. Regardless of nanoribbon geometry, the binding energies of P-doped systems exhibit notable uniformity within the range of  $-8.01$  eV to  $-8.49$  eV, however the adsorption energies in ZGNR are significantly lower than those observed in AGNR. Due to much higher(lower) electron-donating (accepting) capacity of phosphorous(boron) atoms in comparison to 'C' atom, substitutional doping with 'P' or 'B' atoms in AGNR has significant impact on the structural, electronic and adsorption properties of the nanoribbons. We observe that phosphorus doped configurations (edge/center) effectively interact with phosgene molecule with higher adsorption that corresponds to the chemisorption phenomenon. The strongest adsorption energy ( $-8.83$  eV) is obtained for P doped configurations, followed by that for B+P co-doped AGNR ( $-4.23$  eV). These results suggest significantly stronger adsorption of phosgene gas on P doped AGNR than on any other systems reported so far. Band structure analysis estimates that by phosphorus doping, changes in the band gap is significant and it also shows prominent changes in the band structures. Isosurface electronic charge density plots identify that the transfer of charge takes place from graphene system to phosgene molecule. Thus, significant variation in adsorption and electronic properties of P doped AGNR reveal that these geometries immensely promote the detection of phosgene gas, and may be considered as promising chemical sensor for phosgene removal.

UFS

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Physica Scripta  
99 (2024) 3, 035931







# Magnetically reconfigurable toroidal metasurfaces

● N. Acharyya, S. Mallick, S. Rane, M. Upadhyay Kahaly, D. R. Chowdhury

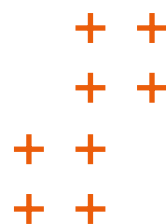
Harnessing electron spin within limited dimensions under applied magnetic fields can lead to spin-assisted tunable light-matter interactions, which form a crucial step in developing frequency-agile opto-spintronic structures toward next generation photonic devices. For this purpose, spin-dependent magneto transport phenomena derived from ferromagnetic (FM)/nonmagnetic (NM) multilayer structures have recently emerged as a useful tool for dynamically tailoring electromagnetic waves. With this pretext, five layers of aluminum (Al)/nickel (Ni) based multilayer thin films in sub skin depth regime are studied in terahertz domain under low-intensity (0 to 30 mT) magnetic fields while systematically varying the NM spacer layer (sandwiched between the FM layers) from 8 to 18 nm. Such thin multi-layer films demonstrate conductivity variations up to  $\approx 40\%$  for 30 mT of applied field. Utilizing the same multilayer configurations, magnetic field induced tunability in a metasurface design is investigated that simultaneously manifests toroidal, dipolar, and other higher-order modes. Further, multipolar analysis reveals that the nonradiative toroidal and radiative dipole modes can be enhanced by almost 56% and 183%, respectively, under 0–30 mT magnetic fields. Such magnetic field-induced simultaneous control over radiative and non-radiative resonances can be pivotal for next generation terahertz magnetophotonic devices.

UFS

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Advanced Optical Materials  
12 (2024) 13, 2303045





# Novel Au/Cu<sub>2</sub>NiSnS<sub>4</sub> nano-heterostructure: Synthesis, structure, heterojunction band offset and alignment, and interfacial charge transfer dynamics

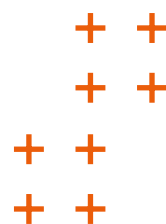
● Y. A. Jadhav, G. K. Rahane, T. Goswami, K. Jagadish, K. Chordiya, A. Roy, T. Debnath, S. B. Jathar, R. Devan, M. Upadhyay Kahaly, S. R. Rondiya, H. N. Ghosh, and N. Y. Dzade

Considering the importance of physics and chemistry at material interfaces, we have explored the coupling of multinary chalcogenide semiconductor Cu<sub>2</sub>NiSnS<sub>4</sub> nanoparticles (CNTS NPs) for the first time with the noble metal (Au) to form Au-CNTS nano-heterostructures (NHSs). The Au-CNTS NHSs is synthesized by a simple facile hot injection method. Synergistic experimental and theoretical approaches are employed to characterize the structural, optical, and electrical properties of the Au-CNTS NHSs. The absorption spectra demonstrate enhanced and broadened optical absorption in the ultraviolet–visible–near-infrared (UV–Vis–NIR) region, which is corroborated by cyclic voltammetry (CV) readings. CV measurements show type II staggered band alignment, with a conduction band offset (CBO) of 0.21 and 0.23 eV at the Au-CNTS/CdS and CNTS/CdS interface, respectively. Complementary first-principles density functional theory (DFT) calculations predict the formation of a stable Au-CNTS NHSs, with the Au nanoparticle transferring its electrons to the CNTS. Moreover, our interface analysis using ultrafast transient absorption experiments demonstrate that the Au-CNTS NHSs facilitates efficient transport and separation of photoexcited charge carriers when compared to pristine CNTS. The transient measurements further reveal a plasmonic electronic transfer from the Au nanoparticle to CNTS. Our advanced analysis and findings will prompt investigations into new functional materials and their photo/electrocatalysis and optoelectronic device applications in the future.

**Kalyani CHORDIYA**  
**Mousumi UPADHYAY KAHALY**

**ACS Appl. Mater. Interfaces**  
**16 (2024) 17, 21746–21756**





# Light-induced photodissociation in the lowest three electronic states of the NaH molecule

● O. Umarov, A. Csehi, P. Badankó, G. J. Halász, and Á. Vibók

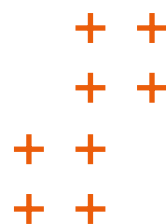
It has been known that electronic conical intersections in a molecular system can also be created by laser light even in diatomics. The direct consequence of these light-induced degeneracies is the appearance of a strong mixing between the electronic and vibrational motions, which has a strong fingerprint on the ultrafast nuclear dynamics. In the present work, pump and probe numerical simulations are performed with the NaH molecule involving the first three singlet electronic states ( $X^1\Sigma^+(X)$ ,  $A^1\Sigma^+(A)$  and  $B^1\Pi(B)$ ) and several light-induced degeneracies in the numerical description. To demonstrate the impact of the multiple light-induced non-adiabatic effects together with the molecular rotation on the dynamical properties of the molecule, the dissociation probabilities, kinetic energy release spectra (KER) and the angular distributions of the photofragments were calculated by discussing the role of the permanent dipole moment as well.

UFS

Ágnes VIBÓK

Phys. Chem. Chem. Phys.  
26 (2024) 7211-7223





# Classical and quantum light-induced non-adiabaticity in molecular systems

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

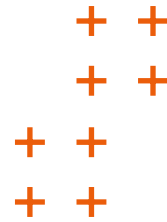
The exchange of energy between electronic and nuclear motion is the origin of non-adiabaticity and plays an important role in many molecular phenomena and processes. Conical intersections (CIs) of different electronic potential energy surfaces lead to the most singular non-adiabaticity and have been intensely investigated. The coupling of light and matter induces conical intersections, which are termed light-induced conical intersections (LICIs). There are two kinds of LICIs, those induced by classical (laser) light and those by quantum light like that provided by a cavity. The present work reviews the subject of LICIs, discussing the achievements made so far. Particular attention is paid to comparing classical and quantum LICIs, their similarities and differences and their relationship to naturally occurring CIs. In contrast to natural CIs, the properties of which are dictated by nature, the properties of their light-induced counterparts are controllable by choosing the frequency and intensity (or coupling to the cavity) of the external light source. This opens the door to inducing and manipulating various kinds of non-adiabatic effects. Several examples of diatomic and polyatomic molecules are presented covering both dynamics and spectroscopy. The computational methods employed are discussed as well. To our opinion, the young field of LICIs and their impact shows much future potential.

UFS

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AVS Quantum Sci.  
6 (2024) 2, 023501





# Competition of multiphoton ionization pathways in lithium

● B. Tóth, A. Tóth, and A. Csehi

We study the three-photon ionization of atomic lithium by intense, short light pulses, via numerically solving the time-dependent Schrödinger equation. Two-photon Rabi oscillations are induced between the 2s and 4s states, which are damped due to single-photon ionization to the p continuum. Developing a minimal three-level model, we analyze the spectral features of the Autler–Townes (AT) doublet that is formed upon the resonant coupling with the laser pulse. Furthermore, we show that this  $2s \rightarrow 4s \rightarrow p$  continuum pathway is the dominant process, if the duration of the laser pulse exceeds a certain value. For shorter pulses, ionization through the 2p state ( $2s \rightarrow 2p \rightarrow 4d \rightarrow f$  continuum) gradually becomes the dominant process, provided that the pulse is strong enough to induce several Rabi floppings. Here, we trace the competition of these ionization pathways by observing the structural changes in the shape of the AT doublet.

UFS

Attila TÓTH

J. Phys. B: At. Mol. Opt. Phys.  
57 (2024) 055002





# Proposal for an electromagnetic mass formula for the X17 particle

● S. Varró

Recent observations of anomalous angular correlations of electron–positron pairs in several nuclear reactions have indicated the existence of a hypothetical neutral boson of rest mass  $\sim 17 \text{ MeV}/c^2$ , called the X17 particle. Similarly, one has interpreted an independent set of experiments on photon pair spectra around the invariant mass  $\sim 38 \text{ MeV}/c^2$ , by assuming the existence of the so-called E38 particle. In the present paper, we derive analytical mass formulas for the X17 particle and the E38 particle, on the basis of quantum electrodynamics. We shall use the exact solutions of the Dirac equation of the joint system of a charged particle and plane waves of the quantized electromagnetic radiation. When these solutions are applied to a proton, they lead to dressed radiation quanta with a rest mass of  $17.0087 \text{ MeV}/c^2$ , which may be identified with the X17 vector bosons. A similar consideration, applied to the odd quarks of the neutron, yields dressed quanta, whose mass equals  $37.9938 \text{ MeV}/c^2$ , corresponding to the E38 particle. These formulas, besides the Sommerfeld fine structure constant and the masses of the nucleons, do not contain any adjustable parameters. The present analysis also delivers the value  $0.846299 \text{ fm}$  for the proton radius.

UFS

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Universe  
10 (2024) 2, 86





# Survival benefit of stereotactic radiotherapy in the complex management of metastatic melanoma

● Gy. Kelemen, Zs. Együd, Á. Dobi, L. Varga, R. Kószó, E. Borzási, V. Paczona, Z. Végváry, F. Borzák, E. Fodor, H. Ócsai, E. Baltás, J. Oláh, and K. Hideghéty

Background/Aim: Targeted therapy and immunotherapy, with additional stereotactic radiation therapy (SRT) have revolutionized the management of metastatic malignant melanoma (mMM). We aimed to analyze the effectiveness and safety of SRT and determine its role in the complex management of mMM. Patients and Methods: We treated 24 patients with solitary metastasis, 15 with oligometastatic disease and one with multiple metastases. The primary endpoint was to investigate the possible effect of stereotactic radiotherapy for metastatic lesions on patients' survival taking the systemic therapy into consideration. Results: The median overall survival (OS) for the entire group was 30.07 months; 50% of them received immunotherapy, 32% received targeted therapy. Complete remission of the irradiated lesions was observed in six patients, partial tumor response was achieved in 13, while stable disease was detected in 10; tumor progression occurred in four cases. Compartmental recurrence (recurrence in the brain in a not previously irradiated region) developed in seven patients. OS was significantly longer in those with extracranial metastases treated with stereotactic body radiotherapy in comparison to brain SRT. We found a strong correlation between tumor response and mean OS (42.5 months after complete or partial remission versus 11.8 months in those with stable or progressive disease). No OS difference was observed according to the number of irradiated lesions or type of systemic therapy before SRT (no therapy: 43.6 months, with therapy: 25.7 months). Significant OS advantage was shown when immunotherapy was administered post-SRT (mean OS: with immunotherapy: 39.6 months, no immunotherapy: 18.5 months). Conclusion: In the case of oligometastatic MM, SRT can be used safely and with good efficiency in addition to targeted therapy/anti-programmed cell death protein 1 therapy. Improved survival warrants including SRT in the complex management of mMM, however, further studies are needed for SRT optimization.

UFS

Katalin HIDEGHÉTY

Anticancer Research  
44 (2024) 1, 205-212





# Few-cycle surface plasmon polaritons

- K. Komatsu, Zs. Pápa, T. Jauk, F. Bernecker, L. Tóth, F. Lackner, W. E. Ernst, H. Ditlbacher, J. R. Krenn, M. Ossiander, P. Dombi, and M. Schultze

Surface plasmon polaritons (SPPs) can confine and guide light in nanometer volumes and are ideal tools for achieving electric field enhancement and the construction of nanophotonic circuitry. The realization of the highest field strengths and fastest switching requires confinement also in the temporal domain. Here, we demonstrate a tapered plasmonic waveguide with an optimized grating structure that supports few-cycle surface plasmon polaritons with >70 THz bandwidth while achieving >50% light-field-to-plasmon coupling efficiency. This enables us to observe the—to our knowledge—shortest reported SPP wavepackets. Using time-resolved photoelectron microscopy with suboptical-wavelength spatial and sub-10 fs temporal resolution, we provide full spatiotemporal imaging of co- and counter-propagating few-cycle SPP wavepackets along tapered plasmonic waveguides. By comparing their propagation, we track the evolution of the laser-plasmon phase, which can be controlled via the coupling conditions.

**UFS**

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**László TÓTH**  
**Péter DOMBI**

**Nano Lett.**  
**24 (2024) 8, 2637–2642**







# Ultrafast surface plasmon probing of interband and intraband hot electron excitations

● P. Sándor, B. Lovász, J. Budai, Zs. Pápa, and P. Dombi

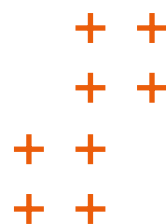
Upon the interaction of light with metals, nonthermal electrons are generated with intriguing transient behavior. Here, we present femtosecond hot electron probing in a novel optical pump/plasmon probe scheme. With this, we probed ultrafast interband and intraband dynamics with 15 nm interface selectivity, observing a two-component-decay of hot electron populations. Results are in good agreement with a three-temperature model of the metal; thus, we could attribute the fast ( $\sim 100$  fs) decay to the thermalization of hot electrons and the slow (picosecond) decay to electron–lattice thermalization. Moreover, we could modulate the transmission of our plasmonic channel with  $\sim 40\%$  depth, hinting at the possibility of ultrafast information processing applications with plasmonic signals.

**UFS**

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**Zsuzsanna PÁPA**  
**Péter DOMBI**

**Nano Lett.**  
**24 (2024) 26, 8024–8029**





# Pt/MnO interface induced defects for high reverse water gas shift activity

- I. Szentı, A. Efremova, J. Kiss, A. Sápi, L. Óvári, Gy. Halasi, U. Haselmann, Z. Zhang, J. Morales-Vidal, K. Baán, Á. Kukovecz, N. López, Z. Kónya

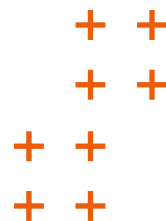
The implementation of supported metal catalysts heavily relies on the synergistic interactions between metal nanoparticles and the material they are dispersed on. It is clear that interfacial perimeter sites have outstanding skills for turning catalytic reactions over, however, high activity and selectivity of the designed interface-induced metal distortion can also obtain catalysts for the most crucial industrial processes as evidenced in this paper. Herein, the beneficial synergy established between designed Pt nanoparticles and MnO in the course of the reverse water gas shift (RWGS) reaction resulted in a Pt/MnO catalyst having  $\approx 10$  times higher activity compared to the reference Pt/SBA-15 catalyst with  $>99\%$  CO selectivity. Under activation, a crystal assembly through the metallic Pt (110) and MnO evolved, where the plane distance differences caused a mismatched-row structure in softer Pt nanoparticles, which was identified by microscopic and surface-sensitive spectroscopic characterizations combined with density functional theory simulations. The generated edge dislocations caused the Pt lattice expansion which led to the weakening of the Pt–CO bond. Even though MnO also exhibited an adverse effect on Pt by lowering the number of exposed metal sites, rapid desorption of the linearly adsorbed CO species governed the performance of the Pt/MnO in the RWGS.

UFS

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Gyula HALASI

Angew. Chem.Int. Ed.  
63 (2024) e2023173





# Hexagonal boron nitride on metal surfaces as a support and template

● L. Óvári, A. P. Farkas, K. Palotás, G. Vári, I. Szent, A. Berkó, J. Kiss, and Z. Kónya

The synthesis and characterization of two dimensional materials are in the focus of nanomaterial and surface science, heterogeneous catalytic and nanoelectronic research laying the basis for various technological applications. Hexagonal boron nitride (h-BN) is an important member of 3D and reduced dimensional materials. Atomically clean  $sp^2$ -hybridized 2D nano-layers can be grown on various metal supports by different chemical and physical vapor deposition techniques. In case of a significant lattice mismatch and a strong interaction at the h-BN/metal interface, a periodically undulating monolayer - a so-called "moiré structure" - is formed. In the present review, we address some important characteristics of h-BN prepared on several metal surfaces, and we focus on its application as a template for individual atoms, metal clusters and molecules. Moreover, several experimental findings are collected about the features and applications of monolayer h-BN nanosheets as supporting materials. We highlight the results of recent surface science studies, which emphasize the unique role of h-BN including nanomeshes in characteristic adsorption properties, stability and catalytic activity. The characterization of few layer and defective h-BN involving their catalytic applications are also the subject of the present review. We present a comprehensive overview on the electronic and vibrational states of nanoparticles (covered by adsorbates, as well) monitored by surface spectroscopy tools, e.g. XPS, ARPES, UPS, LEIS, AES, STS and HREELS. We also elaborate on the structural and morphological information of h-BN nanoobjects obtained by scanning probe microscopy (SPM). It is also highlighted that density functional theory (DFT) is considered as a very important complementary technique contributing to the better understanding of experimental results. Beside updated recollection of key findings, we outline the present and future research directions of 2D materials and their heterostructures including h-BN-based systems.

UFS

László ÓVÁRI  
Arnold P. FARKAS

Surface Science Reports





# Effect of single-crystal $\text{TiO}_2$ /perovskite band alignment on the kinetics of electron extraction

● X. Chen, H. P. Pasanen, R. Khan, N. T. Tkachenko, Cs. Janáky, and G. F. Samu

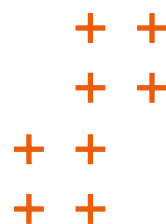
The kinetics of electron extraction at the electron transfer layer/perovskite interface strongly affects the efficiency of a perovskite solar cell. By combining transient absorption and time-resolved photoluminescence spectroscopy, the electron extraction process between  $\text{FA}_{0.83}\text{Cs}_{0.17}\text{Pb}(\text{I}_{0.83}\text{Br}_{0.17})_3$  and  $\text{TiO}_2$  single crystals with different orientations of (100), (110), and (111) were probed from subpicosecond to several hundred nanoseconds. It was revealed that the band alignment between the constituents influenced the relative electron extraction process.  $\text{TiO}_2(100)$  showed the fastest overall and hot electron transfer, owing to the largest conduction band and Fermi level offset compared to  $\text{FA}_{0.83}\text{Cs}_{0.17}\text{Pb}(\text{I}_{0.83}\text{Br}_{0.17})_3$ . It was found that an early electron accumulation in these systems can have an influence on the following electron extraction on the several nanosecond time scale. Furthermore, the existence of a potential barrier at the  $\text{TiO}_2$ /perovskite interface was also revealed by performing excitation fluence-dependent measurements.

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J. Phys. Chem. Lett.  
15 (2024) 2057–2065





# Charge transfer kinetics in halide perovskites: On the constraints of time-resolved spectroscopy measurements

● X Chen, P. V. Kamat, Cs. Janáky, and G. F. Samu

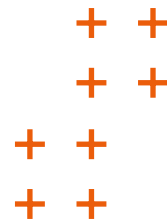
Understanding photophysical processes in lead halide perovskites is an important aspect of optimizing the performance of optoelectronic devices. The determination of exact charge carrier extraction rate constants remains elusive, as there is a large and persistent discrepancy in the reported absolute values. In this review, we concentrate on experimental procedures adopted in the literature to obtain kinetic estimates of charge transfer processes and limitations imposed by the spectroscopy technique employed. Time-resolved techniques (e.g., transient absorption–reflection and time-resolved photoluminescence spectroscopy) are commonly employed to probe charge transfer at perovskite/transport layer interfaces. The variation in sample preparation and measurement conditions can produce a wide dispersion of the measured kinetic parameters. The selected time window and the kinetic fitting model employed introduce additional uncertainty. We discuss here evaluation strategies that rely on multiexponential fitting protocols (regular or stretched) and show how the dispersion in the reported values for carrier transfer rate constants can be resolved.

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ACS Energy Lett.  
9 (2024) 6, 3187–3203





# Au-decorated $\text{Sb}_2\text{Se}_3$ photocathodes for solar-driven $\text{CO}_2$ reduction

● J. M. Ch. M. Dela Cruz, Á. Balog, P. S. Tóth, G. Bencsik, G. F. Samu, and Cs. Janáky

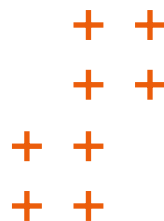
Photoelectrodes with FTO/Au/ $\text{Sb}_2\text{Se}_3$ /TiO<sub>2</sub>/Au architecture were studied in photoelectrochemical CO<sub>2</sub> reduction reaction (PEC CO<sub>2</sub>RR). The preparation is based on a simple spin coating technique, where nanorod-like structures were obtained for  $\text{Sb}_2\text{Se}_3$ , as confirmed by SEM images. A thin conformal layer of TiO<sub>2</sub> was coated on the  $\text{Sb}_2\text{Se}_3$  nanorods via ALD, which acted as both an electron transfer layer and a protective coating. Au nanoparticles were deposited as co-catalysts via photo-assisted electrodeposition at different applied potentials to control their growth and morphology. The use of such architectures has not been explored in CO<sub>2</sub>RR yet. The photoelectrochemical performance for CO<sub>2</sub>RR was investigated with different Au catalyst loadings. A photocurrent density of  $\sim 7.5 \text{ mA cm}^{-2}$  at  $-0.57 \text{ V vs. RHE}$  for syngas generation was achieved, with an average Faradaic efficiency of  $25 \pm 6\%$  for CO and  $63 \pm 12\%$  for H<sub>2</sub>. The presented results point toward the use of  $\text{Sb}_2\text{Se}_3$ -based photoelectrodes in solar CO<sub>2</sub> conversion applications.

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EES. Catal.  
2 (2024) 664-674





# Temperature dependent carrier dynamics in Ga-alloyed CdSe/ZnS core–shell quantum dots

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In this work, temperature dependent transient absorption spectroscopy measurements are presented on gallium-alloyed CdSe/ZnS core–shell nanoparticles between 30 and 130 °C. To our knowledge, temperature dependent measurements in these systems have been reported only in a few papers, although all processes related to carrier recombination are affected by temperature. For these experiments, gallium-alloyed CdSe/ZnS QD samples were used with nominal doping percentages of 2.5%, 7.5%, 15%. The experimental results show that the transient absorption decay is faster for the pristine CdSe/ZnS samples than in the gallium-alloyed samples at all temperatures. It is assumed that Ga-alloying promotes the formation of trions in the samples by introducing occupied impurity levels within the bandgap of CdSe. The resulting Coulomb blockade will, in turn, prolong the hot-electron relaxation process. By variation of the temperature, the distribution of charge carriers in the different recombination channels can be altered to accelerate recombination in the Ga-alloyed samples at higher temperatures. These measurements demonstrated their usefulness for observing the redistribution of charge carriers among different relaxation pathways.

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**J. Phys. Chem. C**  
**128 (2024) 9, 3815–3823**





## Towards a $10^{10}$ n/s neutron source with kHz repetition rate, few-cycle laser pulses

- K. Osvay, L. Stuhl, P. Varmazyar, T. Gilinger, Z. Elekes, A. Fenyvesi, K. Hideghéty, R. E. Szabó, M. Füle, B. Bíró, Z. Halász, Z. Korkulu, I. Kuti, R. Molnár, A. Ébert, R. Polanek, E. Buzás, B. Nagy, P. K. Singh, S. Hussain, Á. Börzsönyi, Zs. Fülöp, T. Tajima, G. Mourou, and G. Szabó

A project has been launched for the development of a laser-based neutron source with the few-cycle lasers available at ELI ALPS. Here we show the first experiments, when deuterons were accelerated from ultrathin deuterated foils at 1 Hz repetition rate with the use of 12 fs, 21 mJ laser pulses. The energy spectra of the accelerated deuterons were measured with Thomson ion spectrometers both in forward and backward directions. The accelerated deuterons induced  $2\text{H}+2\text{H}$  fusion reaction in a deuterated polyethylene disk. The resulting fast neutrons were measured with a time-of-flight (ToF) detector system, within which each detector consisted of a plastic scintillator and a photomultiplier, at four different angles relative to the normal of the neutron converter disk. We found good agreement with the simulated angular distribution and energy spectra. Here, we also present preparations for the next phases when the repetition rate is increased to 10 Hz. The developed flat liquid jet was demonstrated to accelerate protons over 0.6 MeV cutoff energy with a stability better than 4% for 15 min. We developed two further neutron measurement techniques: a liquid scintillator, the ToF signal of which was evaluated with the pulse shape discrimination method, and a bubble detector spectrometer calibrated against a conventional PuBe source. One of the first upcoming applications is the irradiation of zebrafish embryos with laser-generated ultrashort bunch neutrons. As this experiment needs to be implemented in vacuum, the steps of careful preparation and calibration measurements are also discussed.

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