Session: Photonics and Hybrid Materials (PH)
PH-P01 - PH-P07

PH-P01 (Poster)

Influence of co-dopings of alkaline metal ions in Er-doped $CaSnO_3$ on its up-conversion emission intensity

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Up-conversion phosphor, which can emit visible light excited by near infrared radiation, gains great attention, since it is expected to additionally use near infrared region for the generation of electricity by hybridizing with solar cells. It was reported that some types of rare-earth-doped oxides, such as Er/Yb-doped $CaZrO_3$ [1] and $CaMoO_4$ [2], show efficient up-conversion emission by 980 nm excitation and also that up-conversion emission intensity is enhanced by co-doping of alkaline metal ions [3]. However, the mechanism of the enhancement of the up-conversion emission intensity due to co-doping of alkaline metal ions has still remained unclear. In this study, Er-doped $CaSnO_3$ phosphors co-doped with alkaline ions, such as Li, Na, K, Rb and Cs, were synthesized with the conventional solid state reaction method and their crystal structures were characterized by the X-ray diffraction (XRD). The observed up-conversion emission spectra excited by 980 nm irradiation of Na co-doped $CaSnO_3$:Er are shown in Fig. 1 as an example of the current results. From these results, it is confirmed that up- conversion emission intensity is enhanced approx. 5 times by Na co- doping at maximum.

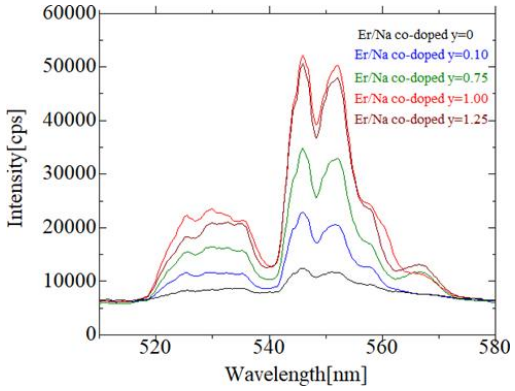

FIG.1 the up-conversion emission spectrumof Na co-doped $CaSnO_3$:Er (x=0.01 in $Ca_{1-x/2}Sn_{1-x/2}Er_xO_3$)

Keywords: up-conversion, CaSnO3, Er, alkaline metal co-doping

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PH-P02 (Poster)

Influence of oxygen ratio on growth and optical properties of ZnO thinfilm prepared by pulse electron deposition method

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Zinc oxide (ZnO) nanocrystalline thin films have been synthesized by pulse electron deposition technique with difference of oxygen ratio. X-ray diffraction (XRD) studies confirm the presence of hexagonal wurtzite ZnO structure in synthesized films. The results show that the lattice constant slightly decreases and the crystal size increases with increasing oxygen concentration. The surface morphology of ZnO films were examined by scanning electron microscope (SEM). Ultraviolet-Visible (UV-Vis) spectroscopic analysis is carried out to calculate energy band gap of the ZnO films. The band gap decreases from 3.89 eV to 3.35 eV when increasing oxygen concentration from 0 to 100%.

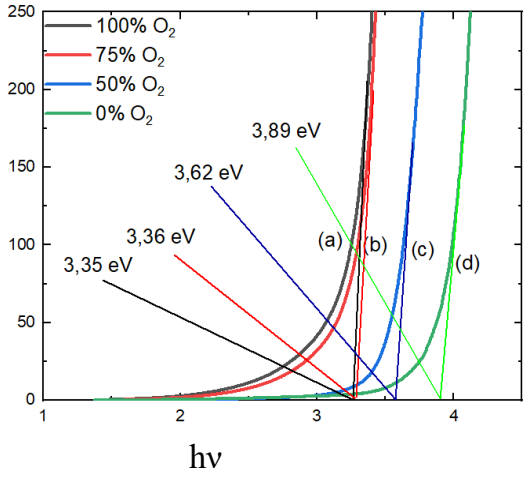

FIG. 1. $(\alpha h\nu)^2$ vs. photon energy ($h\nu$) of ZnO thin films deposited with different oxygen ratio

Keywords: ZnO, nanocrystalline, UV-Vis, band gap

PH-P03 (Poster)

Enhancing the Absorption Figure of Merit on Solution-Based CuO Thin Films by Ni Doping

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We evaluated an absorbance effectiveness on the solar spectrum using an absorption figure of merit (a-FOM) for the conducting thin films. In particular, Ni-doped and un-doped CuO thin films were deposited by a facile and sustainable solution-processed synthesis, whose Ni doping concentration was varied to be 0.2, 0.6, 1, 2, 3, 4 wt.%. We observed a change of smooth surface to an appearance of nanoparticles by Ni doping, which supported to form of a plasmonic mechanism for improving the light capture and retention. The absorption of long wavelengths was improved and extended to the near-infrared range. That is, the bandgap energy decreased from 2.10 to 1.88 eV with Ni doping. Also, we found that the absorption length decreased from 99.93 nm to 63.80 nm as the Ni doping increased. In addition, the CuO-based film with 4 wt.% Ni doping showed a maximal value of a-FOM as high as 30.88 Ω-1cm-1, Corresponding author's to a resistance of 2.07 MΩ/sq and an absorption length of 63.80 nm. Our finding suggested that Ni-doped CuO thin films can be considered as an excellent selection of absorbent conductive oxide layers for application in optoelectronic devices and solar cell systems.

Keywords: CuO, Ni doping, oxide semiconductor, absorption length, absorption figure of merit

PH-P04 (Poster)

Boosting Surface Enhanced Raman Scattering from ZnO/Au Nanorodsby UV excitation

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Surface-enhanced Raman spectroscopy (SERS) has attracted much interest from scientists and engineers because of its potential applications in detection of environmental pollutants, explosives and biomolecules at trace levels. Recently, Photo Induced Enhanced Raman scattering (PIERS) has been reported as a novel technique to further intensify SERS signal under excitation by suitable light prior to or during Raman measurement. In this research, ZnO nanorods were first prepared by galvanic assisted hydrothermal method. Sputtering technique was then applied to fabricate ZnO/Au nanorods. The study showed that Raman signal can be boosted up to 30 times by in situ UV-excitation compared with traditional SERS measurement. This approach provides a robust, fast technique for detection of substances at low concentration.

Keywords: ZnO/Au nanorod; hydrothermal; galvanic; SERS; UV excitation.

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PH-P05 (Poster)

Effect Piezo electric on Surface Enhanced Raman Scattering from ZnO/Au Nanorods

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Surface-enhanced Raman spectroscopy (SERS) has emerged as a very potential tool for sensing toxicants at extremely low concentration. The sensitivity of the SERS substrates depends strongly on the design of noble metal nanostructures. However, optimization of morphology and size of noble metals can only offer a certain enhancement factor. Additional techniques for further boosting Raman signal were studied. In this research, ZnO/Au nanorods were synthesized by hydrothermal and sputtering technquies. The prepared materials can serve as good SERS substrates. Raman scattering can also be intensified efficiently by taking advantages of piezzo electricity of the ZnO/Au material.

Keywords: ZnO/Au nanorod; hydrothermal; galvanic; SERS; piezoelectric...

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EE-P06 (Poster)

Raman-Enhanced Signal of Rhodamine 6G Molecules on SERS Substrate inApplication of Detecting Chemical Residues

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A common Raman spectrometer has not usually detected chemical residues at a lower concentration than 10^{-4} M. However, it can detect them at a lower concentration than10^{-4} M, even lower up to 10^{-9} M with the support of a surface-enhanced Raman scattering (SERS) surface. In this paper, a SERS surface was formed by 5nm-diameter gold nanoparticles (AuNPs) in colloidal solution, and then, randomly deposited on a glass surface to create a SERS/AuNP-layer of 25nm in thickness. A Rhodamine 6G (Rh6G) dye-molecule, deposited on the SERS surface, was used to detect the enhanced Raman amplitude. The Rh6G-solution was diluted at different concentrations, ranging from the concentration from 10^{-4} M to 10^{-9} M. With the same concentration of 10^{-4} M of the Rh6G dye, its typical Raman peaks, deposited on the AuNPs surface, can be clearly detected while these peaks of Rh6G on a flat gold surface could not be seen. Even if the Rh6G solution on the AuNP surface was diluted up to the concentration of 10^{-9}M its typical peaks can still be clearly detected. The significant enhancement of the surface Raman signals at the different concentrations of the Rh6G solution, deposited on the AuNP surface, is due to the roughness of the AuNP surface.

Keywords: Gold nanoparticles (AuNPs), surface-enhanced Raman scattering (SERS), Rhodamine 6G (Rh6G).

PH-P07 (Poster)

Influence of hydrothermal temperatures on characteristics of rare earth upconversion $NaYF_4$ (Yb, Tm) nanoparticles

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In this report, rare-earth upconversion $NaYF_4$: Yb, Tm nanoparticles were fabricated by a simple, low-cost, and high-efficiency method called the hydrothermal method. The characteristics of all samples were investigated by SEM, XRD, FTIR, and PL spectroscopy. The particle size was uniformly around 20 nm in diameter and strongly depended on hydrothermal temperature. When hydrothermal temperatures were controlled from 100ºC to 180ºC, all samples were multi-phases (cubic and hexagonal). And the hexagonal phase prevailed with an increase in the hydrothermal temperature. Furthermore, under 980 nm CW laser excitation, all samples showed PL peaks at 450 nm, 475 nm, and 802 nm Corresponding author's to $^1D_2 \rightarrow {}^3F_4$, $^1G_4 \rightarrow {}^3F_4$, and $^3H_4 \rightarrow {}^3H_6$ transition, respectively. And the highest PL peak intensity can be obtained since the hydrothermal temperature is 180ºC. The results indicated that emission characteristic of the material strongly depends on the phase that can be controlled by the hydrothermal temperature.

Keywords: rare-earth nanoparticles, upconversion nanoparticles, hydrothermal temperature, photoluminescence, $NaYF_4$: Yb, Tm

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PH-P08 (Poster)

Chiropticality of magnetoplasmonic nanoparticle-doped titania hydrogels and aerogels

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Aerogel is a type of solid-phase material formed by the coordinated networking of organic or inorganic matters, which result in an open and highly porous structure. In this study, ultralight, magnetic translucent aerogel monoliths were fabricated from trizma-functionalized anatase (TiO2) and magnetoplasmonic core/shell gold-magnetite composite nanowires (Au@FexOy MagPlas NWs). The resulting aerogel weigh only 0.13 grams per cubic centimeter and possess UV-visible broad absorption, which were modulated by the amount of doped MagPlas NWs. The combination between highly UV-absorbing TiO_2 anatase and magnetoplasmonic core-shell nanowires allows utilization of both UV- and visible spectrum range of light, which potentially enhances the light-harvesting efficiency and photocatalysis applications. Furthermore, the magnetic susceptibility of the gold-magnetite nanowires also allows unique arrangements in TiO2 hydrogels, which opens up possibilities for self-assembly into unique linear and helical superstructures.

Keywords: magnetoplasmonic, nanosynthesis, nanowires, chiral, structural color

FIG. 1. Schematics of the solvent-triggered self-assembly process and images of the synthesized TiO_2 and TiO_2/MagPlas NWs

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Session: Spintronic materials and Devices (SD)
SD-P01 - SD-P10

SD-P01 (Poster)

Gate-Tunable Photodetector and High-Mobility Ambipolar Transistor

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High-quality channel layer is required for next-generation flexible electronic devices. Graphene is a good candidate due to its high carrier mobility and unique ambipolar transport characteristics but typically shows a low on/off ratio caused by gapless band structure. Here we propose a graphene/$MoSe_2$ channel layer with high-k ion-gel gate dielectric. The graphene/$MoSe_2$ device shows both high on/off ratio and carrier mobility. Most importantly, it reveals ambipolar behaviors which are controlled by external bias, although such ambipolarity has never been previously reported in graphene/semiconductor barristor structures. Therefore, our graphene/$MoSe_2$ barristor with ion-gel gate dielectric can offer various with high performances. Here we make a contact of graphene and $MoSe_2$. The graphene/ $MoSe_2$ barristor exhibits high on/off ratio of 104 and high mobility. The modulation of graphene's Fermi level (E_F) by applying gate voltage (V_g) is confirmed by the change in Schottky barrier height at the graphene/$MoSe_2$ junction. Such field effects including ambipolar behaviors are locally investigated by using scanning photocurrent microscopy (SPCM). We have shown that graphene/$MoSe_2$ barristor can be created to obtain highly efficient photocurrent generation and photodetection. Therefore, our graphene/$MoSe_2$ barristor with ion-gel gate dielectric can be a suitable candidate for a ambipolar transistor (with high mobility and on/off ratio) and gate tunable broad-area photodetector (with high EQE and responsivity)..

Keywords: Gate-tunable, photodetector, ambipolar transistor, high mobility, graphene, barristor

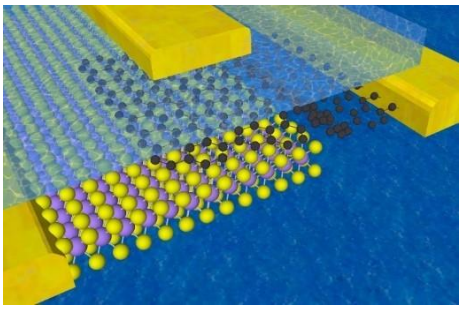

FIG. 1. Graphene/$MoSe_2$ barristor characterization. Schematic diagram

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SD-P02 (Poster)

Neuromorphic devices based on the electrochemical metallization in the ferroelectric material

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The neuromorphic computing system aims to implement artificial neural networks (ANNs), which emulates biological neural networks composed of a large number of neurons massively interconnected by even larger number of synapses. Although several types of architectures have been used to demonstrate ANNs, artificial neurons and synapses have been separately developed by using a wide veriety of meterials and processes, leading to limited scalability, complex suructures and processes, and high cost. If both artificial neurons and synapses can be simultaneously implemented by using electrochemical metallization (ECM) memristors with an idetical electrolyte layer, they can become simplified fundamental building blocks in the design and fabrication of large-scale ANNs for future reconfigurable neuromorphic system. Here, we deomonstrated the simultaneous implementation of artificial neurons and synapses in ECM memristors with an identical electrolyte layer, which ar Ag, Cu, and Ni/$PbZr_{0.52}Ti_{0.48}O_3$(PZT)/$La_{0.8}Sr_{0.2}MnO_3$(LSMO) with an ultrathin ferroelectric PZT layer (~ 5nm). We introduced polarization bound charges of the ferroelectric layer for more controllable cation migration and set-process in an ECM memristor. The Ag/PZT/LSMO showed abrupt and volatile resistive switching caused by the high velocity of the cation migration and could emulate integration-and-fire with stochastic behavior and auto-recovery with low energy comsumption. In contrast, the Ni/PZT/LSMO revealed gradual and non-volatile resistive switching due to the low velocity of the cation migration and could emulate synaptic plasticity with very low variability. Thus, our identical electrolyte-based system could provide an importantstep towards developing large-scale ANNs with high scalability, simple structure, and low cost.

Keywords: Electrochemical metallization, Ferroelectric, Synaptic device, Neuron device

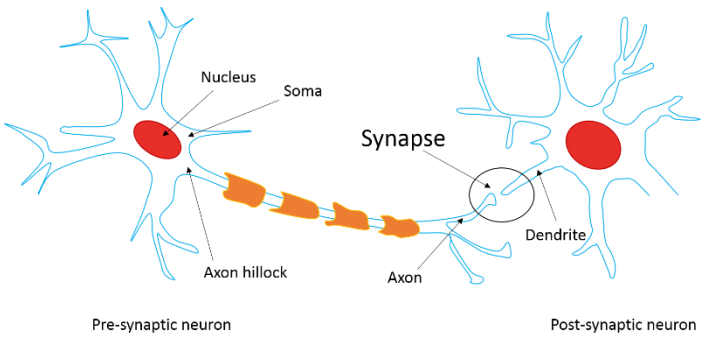

FIG. Schematic image of the biological neuron and synapse structure

SD-P03 (Poster)

Thermoelectric properties of magnesium tinalloy thin films

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In this work, magnesium tin (Mg-Sn) alloy thin films was synthesized in form of low-dimension structure by using magnetron co-sputtering in pure Ar plasma atmosphere. The formation of alloy Mg-Sn thin films was confirmed by X-ray diffraction. The thickness and morphology of the films were obtained from field-emission scanning electron microscopy. The thermoelectric properties of the films were investigated in the temperature range of 50 – 300ºC. The results showed that the films had p-type semiconducting characterization, with some potential thermoelectric average values: electrical conductivity of 420 S/cm, Seebeck coefficient of 41.3 μV/K, and power factor of 72.4 $\mu W/mK^2$. Specifically, the alloy films had a high value of hole mobility of 51.1 cm^2/Vs Corresponding author's to a hole concentration of 2.4×10^{19} cm^{-3} measured at room temperature. These results are very potential for high-performance thermoelectric thin-film applications, especially in low-temperature range.

Keywords: Thermoelectrics, magnesium tin, magnetron co-sputtering, thin films

SD-P04 (Poster) **CANCEL**

~~Investigation the THz frequencies induced from the damping oscillations of electron velocity by ensemble Monte-Carlo simulations in p-i-n GaAs semiconductor device~~

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In this work, we introduce the investigation of damping oscillations of electron velocity in the p-i-n GaAs semiconductor device without external electric field. The variation of electron velocity depends on the internal electric field which is originated from the photoexcited carriers in the device caused by superfast laser pulses with a 12 fs duration at the center photon energy of 1.49 eV. The results show that, in the small size of a few hundred nanometers, the damping oscillations of the velocities are clearly observed and their frequency can be easily determined by fast Fourier transform technique. The special thing is that the frequency strongly depends on the device size and follows the certain rule. In order to derive this rule, we use the regression technique with the data of frequency and size at each carrier concentration and sample temperature. From the obtained results, we expect to find other relations of THz radiations caused by the plasma oscillations in this sample device.

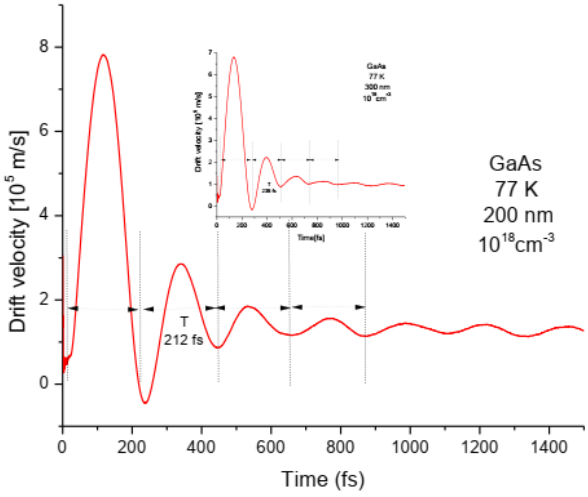

FIG. 1. Drift velocity of electron as a function of time when the device size is 200nm and 300 nm at temperature 77 K.

Keywords: Damped oscillation, EMC simulations, p-i-n structure, THz radiation

SD- P05 (Poster)

Design and fabrication of wireless contactlessliquid level sensor based on LC passive circuit

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In this research, a wireless contactless liquid level sensor has been designed and fabricated based on LC passive resonant circuit with low-cost and small size. The fabricated sensor includes of a contactless parallel electrode capacitor and a planar spiral inductor used as the reader coil. The principle of LC passive circuit is based on LC resonant circuit shown as in Fig.1a, in which the resonant frequency expressing as [1]:

$$f_{res} = \frac{1}{2\pi\sqrt{LC}}$$

where L and C are inductance and capacitance of LC passive circuit, respectively. In this sensor, capacitance C changes due to the vary of liquid level leading to a drift of the resonant frequency. This drift in resonance frequency can be estimated through analyzing the reflection coefficient S11 monitored by using reading coil connected to network analyzer system [2]. Fig.1b showed the reflection coefficient S11 when level of pure water changed from 0 to 175 mm. when the water level increased from 0 to 175 mm, the estimated resonant frequencies decreased from 39.8 down to 22.8 MHz. Based on two parallel capacitor model for this sensor, the linear dependence of $1/f_{res}^2$ vs. water level was investigated and shown as Fig.1c with a high correlation factor of R^2=0.995. The sensitivity of sensor was estimated to be $7.39 \times 10^{-6}\ MHz^{-2}/mm$. Because of contactless, low-cost, small size and easy fabrication, this sensor is potential candidate for using in liquid level measurement of harsh environments such as oil liquid, toxic liquid, acid solution, etc..

Keywords: LC wireless passive, contactless liquid level measurement, wireless contactless sensor, LC passive resonant circuit

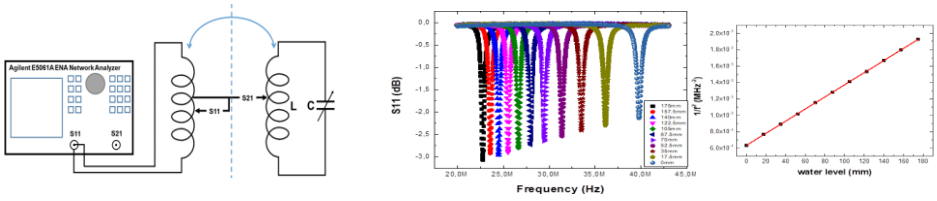

FIG. 1. (a) Principal sensor operation. (b). Reflection coefficient S11 vs. water level. (c) Linear dependence of $1/f_{res}^2$ vs. water level

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SD-P06 (Poster)

Plasma-assisted exfoliation of graphene from graphite: Is graphene truly exfoliated?

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Graphene is an amazing material, inhibiting vast superior properties with numerous applications ranging from environmental treatment, concrete reinforcement, and energy. Among two approaches to graphene making: bottom-up from gaseous or liquid carbon- based precursors and top-down from graphitic sources, synthesising graphene directly from graphite remains the key method for industrial scale-up due to its availability, low cost, and large quantity of products per production. Chemical and mechanical exfoliation have dominated the graphite-to-graphene synthesis pie; however, irradiation exfoliation, particularly plasma-assisted electrochemical exfoliation, has been reported as a promising methodology for graphene synthesis in many recent works due to its novelty, ease of setup, and lack of toxic byproducts. Herein, in this talk, we will discuss how graphene is made from the so-called plasma-assisted "exfoliation“ process, and the mechanism of exfoliation for arc discharge in both air and liquid media.

Keywords: graphene, plasma, electrochemical process, exfoliation, arc discharge.

SD-P07 (Poster)

Ultrafast and Processional Magnetization Dynamics in magnetic tunneljunctions (MTJ) for neuromorphic computing

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We develop new Magnetic Tunnel Junction (MTJ) layer-stacks with low energy requirements, thus, low critical current or in other words low oscillation threshold. The structures of the stacks are 5Ta/ 50CuN/ 5Ta/ 50CuN/ 5Ta/ 5Ru/ 6IrMn/ 2CoFe30/ 0.825Ru/ 2.6CoFe40B20/ MgO/ 2.0CoFe40B20/ 0.21Ta/ 6CoFeSiB/ 2Ta/ 4Ru (Si-MTJ) and 5Ta/ 50CuN/ 5Ta/ 50CuN/ 5Ta/ 5Ru/ 6IrMn/ 2CoFe30/ 0.825Ru/ 2.6CoFe40B20/ MgO/ 2.0CoFe40B20/ 0.21Ta/ 7NiFe/ 2Ta/ 4Ru (Py-MTJ), all thicknesses are in nm. The aim is to manipulate the oscillation via optical access, in our laboratory by using femtosecond laser pulses on the route towards ultrafast spintronics. In our study, the oscillation frequency and effective damping parameters are investigated by using the time-resolved magneto-optical Kerr effect (TRMOKE) microscope as a function of the intensity and direction of the external magnetic field, the intensity of the pump, and cap layer thicknesses. We have shown that by changing the thickness of the capping layer Ta from 2-10nm and fixed Ru 4nm, there is no significant change in the oscillation frequency and effective damping constant. Our results show the temperature difference between cap layer and magnons in magnetic layers is the driving force for spin current generation by ultrafast demagnetization. This study paves the way for developing ultrafast spintronic devices for data storage and information processing. The research is part of the FET-open project SpinAge to develop neuromorphic chips. The final neuromorphic chip designed within the SpinAge consortium device will combine optical access, memristive parts and to spintronic oscillators in one neuron mimicking device. The work has received funding from the European Union's Horizon 20220 research and innovation program under grant agreement No. 899599 (project SpinAge).

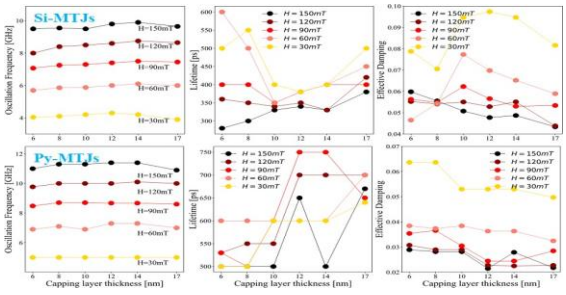

FIG. 1. The precession frequency, lifetime, and effective damping constant as a function of cappinglayer thickness and external magnetic field H.

Keywords: Magnetic Tunnel Junctions, TRMOKE, neuromorphic computing

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SD-P08 (Poster)

Charge Trapping Memory Device Based on Heterostructure of MoS_2 FET and $CrPS_4$

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Atomically thin two-dimensional (2D) materials have emerged as promising candidates for flexible and transparent electronic applications. Here, we introduce non-volatile charge trapping memory devices, based on the 2D heterostructure field-effect transistor consisting of a few-layer MoS_2 channel and $CrPS_4$ charge-trapping gate stack. Clockwise hysteresis behaviors in transfer curves measured at room temperature show a strong dependence on the thickness of CrPS4, which are attributed to charge trapping at trap sites in the $CrPS_4$ layers [1]. Our heterostructure memory device with 75 nm thick $CrPS_4$ layer exhibits both large memory windows up to 99.7 V and high on/off current ratio ($3x10^5$) with good endurance during 625 cycles. Also, non-volatile memory property is obtained because of its excellent trapping ability of trap sites in the $CrPS_4$. Especially, the memory window size can be effectively tuned from 7.6 V to 99.7 V with high on/off current ratio by changing the sweep range of back gate voltage from 10 to 60 V at drain voltage, VD=0.1 V as shown in Fig. 1. Such high performances of the charge trapping memory device with a simple heterostructure provide a promising route towards next-generation memory devices utilizing 2D materials [2].

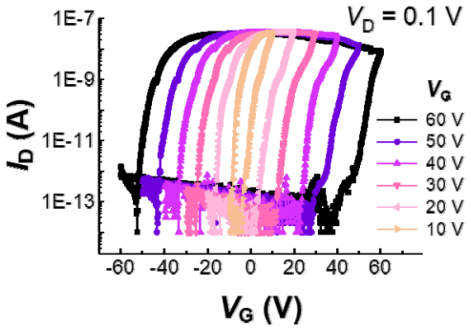

FIG. 1. Transfer characteristics of MoS2 FET on bulk-like CrPS4 with different sweeping range of VG from 10 V to 60 V at VD = 0.1 V

Keywords: Heterostructure, 2D materials, MoS_2, $CrPS_4$, TMDC, TMPS, FET, Memory

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SD-P09 (Poster)

Development of the high sensitive measurement system to investigate the characteristics of magentic fluids

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In this paper, a very high magnetic field-sensitive measurement system based on a giant magnetometer resistance (GMR) sensor was developed to determine the relationship between the magnetization of superparamagnetic nanoparticles (SPMNPs) in the liquid and the excitation magnetic field. The microfluidic device was integrated includes a microfluidic channel with a modified GMR sensor (bonded to a printed circuit board). It was placed in a highly uniform magnetic field that was generated by two Helmholtz coil pairs, which emit magnetic fields in perpendicular directions to magnetize the SPMNPs and define a linear working point for the GMR sensor. The system was used to determine the induced magnetic field of superparamagnetic nanoparticles (BSPMNPs) under the excitation magnetic field. The induced magnetic field, BSPMNPs, was used to calculate the magnetization of the SPMNPs, M, based on the construction of the measuring system and the excitation magnetic field. The proposed system was investigated using superparamagnetic-Fe_3O_4 fluids with diameter of 60 nm, saturation magnetization of 60 emu/g and a concentration of 4.64 mg/mL. A sine wave excitation magnetic field with a frequency of 25 Hz and a variable amplitude in the range of 0–25.7 G was used to magnetize SPMNPs. The results show the properties of SPMNPs were measured by the proposed measurement system and the vibrating sample magnetometer (VSM) system. This method allows to measure the magnetic properties of SPMNPs in liquid instead of measuring on dry samples like the two traditional methods, VSM and PPMS (physical property measurement system).

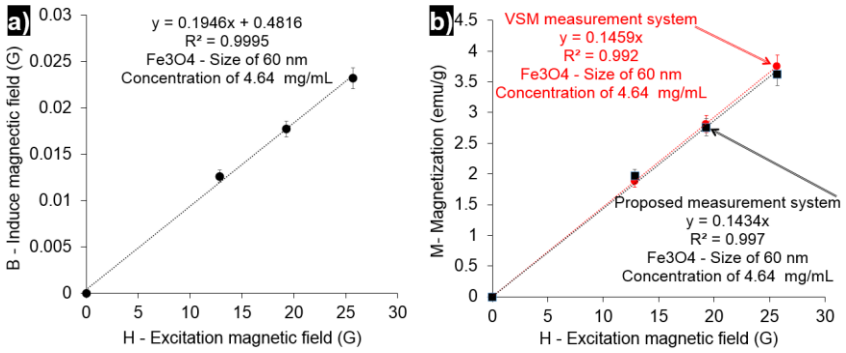

FIG. 1: a) The relationship between the induced magnetic field of SPMNPs in the liquid and the excitation magnetic field was measured by the proposed

Keywords: GMR, microfluidics, Fe_3O_4, magnetic fluids

SD-P10 (Poster)

Fabrication of the Ion-selective Field-effect transitor array for determine the pH of solutions

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The research on fabrication of the Ion-Selective Field-effect transistor (ISFET) array by using microelectronic technology and apply for determine the pH of solutions was described on this paper. The ISFET array was designed and fabricated as below: the structure and mask of ISFET was designed by MEMSCapro software based on SCANA design rule; the shape of transistor was employed by UV-lithography technique, the electrodes and connect film was deposited by sputtering method, the gate electrode was fabricated by SiO2-oxidation technique, the SOG/SOD method was used to dope the n+ region, the wire bonding and packaging technique was used on this project. The ISFET array was successfully developed with 8 transistor on chip, the width/length of gate electrode is 16μm/6μm and the thickness is 6nm. The characteristics of the transistor array was investigated by using Keithley 420SCS Instrument; the threshold voltage was -0.7V with IDSmax = 1mA. The pH sensitive characteristic of the developed transistor was surveyed on range of 2-12 and the sensitivity of sensor was 16mV/pH with LOQ is lower than 0.05 pH, LOD = 0.01pH. The pH sensor was tested with the solutions of some lake in Hoa Binh province (such as: Hoa Binh hydropower reservoir, Chau – Da Bac Lake, Tinh-Da Bac Lake) with the high reliability and low RSD. The obtained results have opened up the possibility of developing compact - fast - real-time and reliable analytical systems to meet the needs of analysis in seafood production and environmental monitoring in Vietnam.

Keywords: Ion-selective field-effect transistor, pH, array sensor, Microelectronics technology

Session: Theory and Computation (TC)
TC-P01 - TC-P07

TC-P01 (Poster)

Water molecular behavior at solid/liquid interfaces examined by *ab initio* molecular dynamics

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Solid/liquid interfaces are ubiquitous in nature and the understanding of their atomic-level structure is crucial for elucidating the atomic mechanism behind reactions occurring on interfaces. Hydrogen evolution reaction (HER) is one of them, which is the dominating process of producing hydrogen upon using as clean energy. Furthermore, a preceding study has found the behavior of water molecules near the catalyst surface does influence the efficiency of HER[1]. Thus, in this study, we used ab initio molecular dynamics (AIMD) simulation in order to figure out the behavior of water molecules and possible influence on the detailed mechanism behind the reaction. Here, we modelled three kinds of solid/liquid interfaces with different solid phases. The first two are pure metals: Pt and Au, which are well-known as highly efficient HER catalysts. The third one is MoS_2, a newly known low-cost promising candidate for HER catalyst [2] with totally different interfacial features. Then, we carried out AIMD simulation to statistically analyses the behavior of water molecules on different interface models.

It turns out in all three models that the water density shows two peaks near the interface, which reveals the extraordinary molecular behavior. To investigate the details, we calculated (1) the angle between the O–H bond of water and the surface normal and (2) the angle between the water bisector and the surface normal of the interfacial water. Finally, the results show the distinct difference of molecular behavior between water on the metals and those on the MoS_2

Acknowledgments: This work was supported by JSPS Grant-in-Aid for Scientific Research on Innovative Areas ‘Crystal Defect Cores’ (JP19H05786, JP20H06195) and Scientific Research (20K05062).

Keywords: solid/liquid interface, AIMD simulation, MoS_2

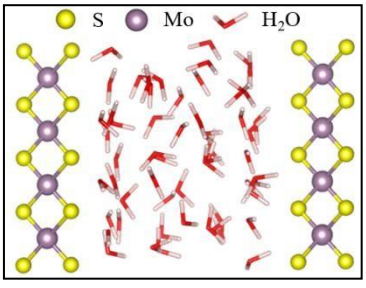

FIG. 1. MoS_2/water interface model

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TC-P02 (Poster)

Extraction of local structural information from X-ray absorption spectra: machine learning approaches

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X-ray absorption spectroscopy (XAS) is a useful technique for characterizing local atomic and electronic structures in materials. Theoretical fingerprint matching based on first-principles calculations is the most quantitative method for extracting local structures and local electronic states from XAS experimental spectra[1]. Recently, machine learning approaches have been proposed to predict XAS from atomic structures to avoid the high computational cost of first-principles calculations. The results are being obtained in research on predicting XAS spectra from given information of atomic structures[2]. Attempts have also been made to extract physical properties such as bond distances, ionic bonding properties, and radial distribution functions from XAS spectra. However, no machine learning model that predicts three-dimensional local atomic structure from XASspectra.

In this work, we constructed machine learning models to predict structural descriptors that numerically represent the atomic structures in three dimensions. The neural network models that predict radial distribution functions (RDF) and orbital-field matrix (OFM)[3], which is a descriptor that deals with the anisotropy of the local structure, the valence electron number of the ligand, and orbital information, were constructed. We used more than 120,000 O K-edge XAS spectra data from the Materials Project database as the training data set. We successfully constructed models that roughly predicted radial distribution functions with 80.4% of the test data. Furthermore, the model that predicted OFM also captured an overview of OFM in 83.0% of the test data. These results demonstrate that the atomic structural information can be directly extracted from XAS spectra by using neural network models.

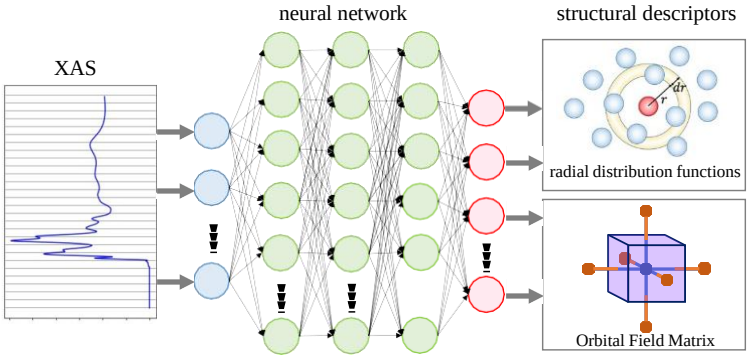

FIG. 1. Schematic representation of the neural network for predicting structural descriptors from XAS spectra

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TC-P03 (Poster)

First-principles study on hydrogen adsorption and dissociation on Palladium clusters embedded in Zr-UiO-67 metal-organic frameworks

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Hydrogen storage via hydrogen spillover effects is the key to enhancing storage capacity at room temperatures [1, 2]. Palladium clusters have been widely known for their efficiency to dissociate hydrogen molecules into hydrogen atoms for spillover activation [2]. Embedding palladium clusters on metal-organic frameworks (MOFs) is important in practical manipulations [3, 4]. In this work, we incorporate palladium clusters (Pd_n, n=1-4) into both the pristine and defective UiO-67 MOF structures to investigate the influence of the interaction between palladium clusters and host materials on hydrogen adsorption and dissociation. Results from density functional theory calculations (DFT) showed that the binding energies per palladium atom are higher in the pristine structure than that in defective ones because palladium clusters prefer chemical binding to the benzene linkers of the pristine instead of the metal nodes in the defect. The hydrogen adsorption energies on Pd_n embedded in pristine UiO-67 are increasing with the cluster sizes, in a range from 0.20 eV to 0.80 eV, while that trend is reversed for the adsorption on free Pd_n clusters and Pd_n embedded in defective UiO-67. It is predicted that the strong bindings of Pd_n with linkers in pristine UiO-67 suppress the electrostatic interaction of the clusters with hydrogen molecules. The dissociation of hydrogen molecules occurs easily without energy barriers on both free Pd_n clusters and Pd_n embedded in defective UiO-67, with n=2 and n=3, while it remains in molecular form for Pd_n in the pristine structures. The dissociation energy barriers for n=4 are comparable for all studied structures, i.e, in a range from 0.18 eV to 0.38 eV. The findings reveal that hydrogen adsorption energies on palladium clusters are notably affected by the incorporation of metal clusters on different host materials, but the dissociation energy barriers are less influenced.

Keywords*:* palladium clusters, metal-organic frameworks, hydrogen dissociationbarriers, first-principles calculations

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TC-P04 (Poster)

Novel Few-layer Nanosheets from Layer Structured Gallium Chalcogenides: Structural, Electronic and Mechanical Properties

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The low-dimensional gallium chalcogenide group semiconductors have recently emerged as interesting candidate materials for the tailoring of two dimensional (2D) layered structures due to their intriguing optical and electronic properties derived by the van der Waals bonding between layers. Herein, two novel series of few-layer nanosheets from gallium sulphur binary compound Ga_2S_3 and Ga_2S_5 are proposed. We have performed the first principle calculations on the structural, electronic and mechanical properties of suggested nanosheet series, to investigate the effects of structural modification and sheet thickness on their structural, electronic, and mechanical properties. Optimized geometries, formation energy, phonon spectra, electronic band structure, and elastic tensor calculation has ensured the energetically, dynamical and mechanical stability for the nanosheets. Furthermore, the theoretically found nanosheet series possess an direct band gap which are different from the well known GaS nanosheet series. These highly anisotropic semiconductor nanosheet series and their derivatives are expected to have broad applications in photocatalysis, and new generation nanoelectronic devices.

Keywords: Nanosheet, DFT, Gallium Chalcogen, structure prediction

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TC-P05 (Poster)

Magneto-optical absorption in a borophene monolayer with titled Dirac cones: Effect of electron - optical phonon coupling

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Two-dimensional (2D) Dirac materials have extraordinary properties and numerous potential applications. 8*Pmmn*-borophene is a 2D Dirac material with titled Dirac cones that promise many interesting optical transitions. In this work, we theoretically investigated the magneto-optical absorption properties in a monolayer 8*Pmmn*-borophene placed in a perpendicular static magnetic field and an electromagnetic wave. Utilizing the perturbation theory, the absorption coefficient (AC) was calculated considering the electron - optical phonon scattering. The resonant absorption peaks were observed in the absorption spectra. The dependence of the full width at half maximum of resonant peaks on the magnetic field and temperature was obtained. Effect of the titled Dirac cones was also considered by via the polarity of the AC verus valley indices. The obtained results are the basis for further studies on the applications of borophene to nano-optoelectronic devices and valleytronics.

Keywords: magneto-optical absorption; absorption coefficient; electron – phonon coupling; Dirac material; borophene

TC-P06 (Poster)

Controllable electronic properties and contact types of metal/semiconductor MoSH/$MoSi_2N_4$ heterostructure

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Following the successful synthesis of single-layer metallic Janus MoSH and semiconducting $MoSi_2N_4$, we investigate the electronic and interfacial features of metal/semiconductor MoSH/$MoSi_2N_4$ van der Waals (vdW) contact. We find that the metal/semiconductor MoSH/$MoSi_2N_4$ contact forms p-type Schottky contact (p-ShC type) with small Schottky barrier (SB), suggesting that Janus MoSH can be considered as an efficient metallic contact to $MoSi_2N_4$ semiconductor with high charge injection efficiency. The electronic structure and interfacial features of the MoSH/ $MoSi_2N_4$ vdW heterostructure are tunable under strain and electric fields, which give rise to the SB change and the conversion from p-ShC to n-ShC type and from ShC to Ohmic contact. These findings could provide a new pathway for the design of optoelectronic applications based on metal/semiconductor MoSH/$MoSi_2N_4$ vdW heterostructures [1].

Keywords: Electronic properties; First-principles calculations; van der Waals heterostructures; Contact types.

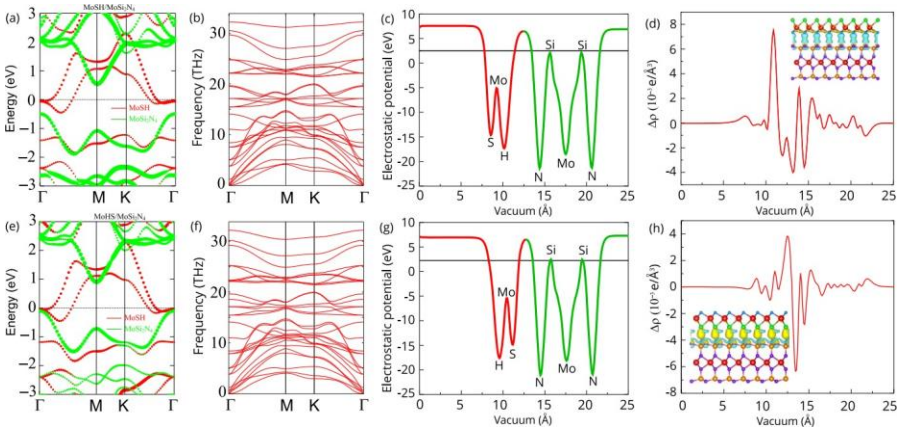

FIG. 1. (a and e) Orbital-projected band structures, (b and f) phonon dispersion curves, (c and g) plane-averaged electrostatic potentials, and (d and h) planar average charge density differences of MoSH/$MoSi_2N_4$ and MoHS/$MoSi_2N_4$ HTSs. The MoSH and $MoSi_2N_4$ layers are separated by red and green circles, respectively. The charge accumulation is depicted by yellow, and the charge depletion is illustrated by cyan.

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TC-P07 (Poster)

Quantum theory of the effect of increasing weak electromagnetic waveby a strong laser radiation in 2D Graphene

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Analytic expressions for the absorption coefficient (AC) of a weak electromagnetic wave (EMW) in 2D Graphene under influence of a strong laser radiation are calculated using the quantum kinetic equation for electrons in the case of electron-optical phonon scattering. The dependence of the AC on the intensity E_{01} and the frequency Ω_1 of a weak EMW , on the intensity E_{02} and the frequency Ω_2 of a strong laser radiation , on the temperature T of the system and on the parameters of 2D Graphene is obtained. The numerical results show that the AC of a weak (EMW) in 2D Graphene can have negative values. This demonstrates the possibility of increasing weak electromagnetic wave by a strong laser radiation in 2D Graphene **.**This is different from the similar problem in bulk semiconductors and from the case without strong laser radiation.

Keywords: absorption coefficient, electromagnetic wave, 2D Graphene, quantumkinetic equation