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Agnieszka Czyżowska (OMRF, Oklahoma, USA)
Dinh Xuan Anh Tuan (Université de Paris, Paris, France)
Ewa Durska (UW, Warsaw, Poland)
Ladislav Havela (CUNI, Prague, Czech Republic)
Nguyen Thi Ngoc Anh (IMS-VAST, Hanoi, Vietnam)
Nguyen Hung Son (UW, Warsaw, Poland)
Nguyen Thi Thu Thuy (HCMUC, HCM city, Vietnam)
Phan Anh Tu (VNUHCM-USSH, HCM city, Vietnam)
Zbigniew Tarnawski (AGH, Cracow, Poland)
Trinh Xuan Hoang (IOP-VAST, Hanoi, Vietnam)

#### **HONORARY GUESTS**

Robert Stawarz (Vice-Rector PUC, Cracow) Doan Dinh Phuong (Director IMS-VAST, Vietnam) Dawid Nałęcz (Vice-Director IF-PUC, Cracow) Tran The Hung (Director IAE-QBU, Vietnam)

#### **VENUE**

for the onsite meetings

Pedagogical University of Cracow (PUC), Podchorazych 2, 30 084 Krakow Lecture hall: 110N (WVSP2021) Lecture hall: 111N (PolVietSym2021)

#### Links for the online meetings in MS Teams

E-mail: wvsp2021@up.krakow.pl

Website:

https://wvsp2021.up.krakow.pl/the-sixth-workshop-of-vietnamese-students-in-poland-wvsp2021/

Link Facebook (in Vietnamese):

https://www.facebook.com/H%E1%BB%98I-TH%E1%BA%A2O-WVSP-2021-100248162393660

E-mail: polvietsym2021@up.krakow.pl

Website:

https://wvsp2021.up.krakow.pl/the-second-poland-vietnam-symposium-polvietsym2021/





QR code of WVSP21021

QR code of PolVietSym2021 (reading the website by a device camera with Google Lens app)

#### WEBSITE MANAGER

Nhu-Tarnawska Hoa Kim Ngan

#### FACEBOOK ADMISTRATORS

Nguyen Thi Thu Ha Nguyen Thi Hue

### PROGRAM of WVSP2021 and PolVietSym2021

The two onsite meetings are in lecture halls 110N and 111N with the participants being present in Cracow.

All presentations will be shown online.

Friday, November 19, 2021 (all hours are given in CET (UTC+2))			
(an nours are given in CE1 (O1C+2))			
		the Organising Committee	
		onsite meetings:	
16:00-18:00		PUC), Podchorazych 2, 30-084 Krakow.	
10.00 10.00		110N and 111N	
		main entrance from Chmiela street	
	(see map_Krakow-Ry	nek-PUC in the website)	
	Saturday, November	20, 2021	
	_	ng Session	
		nline meeting: Enter here	
	_	Nhu-Tarnawska, Mai Suan Li,	
		ej Kornaś	
		ne address	
		Honorary guests of WVSP2021: <b>Robert Stawarz</b> , Vice-Rector of the Pedagogical University of Cracow	
		Institute of Materials Science, Vietnam	
10:00:10:15	Academy of Science and Technology		
	<b>Dawid Nałęcz</b> , Vice-Director of Institute of Physics, Pedagogical University		
	of Cracow		
	Tran The Hung, Director of the Institute of Agriculture and Environment,		
	Quang Binh University, Vietnam	101	
		ence and Culture	
		nline meeting: Enter here m Ngan Nhu-Tarnawska	
		av Havela	
10:15-11:00	Hydrogen storage in metal hydrides – fundamental principles meet practical life		
	PL-1		
	Nguyen T	hi Thu Thuy	
11:00-11:30	The values in Vietnamese Mother Worship		
		I-1	
11:30-11:50	Coffee/tea break		
	Session 2A Materials Science	Session 2B Natural Science-1	
	Lecture hall 110N  Online meeting: Enter here	Lecture hall 111N.  Online meeting: Enter here	
	Chairman: Tran Vinh Hung	Chairman: Ladia Havela	
	Chairman, Tran vinn Trung	Chamman, Ladia Havela	

	Thi Ngoc Anh Nguyen	Ewa Durska
	1/f noise characterization of MgO-	The power of plants – application of
	based magnetoresistive sensors	fossil spores and pollen grains
11:50-12:20	enable a noise-based technique for	in geology
	detecting of weak magnetic signals	3.2.2.87
	I-2	I-4
	Thi Hue Nguyen	Thiep Vo Van
	Effective generation of optical	Assessment of the risk of Lead
12:20-12:30	vortex beams using flat-surface	exposure when consuming Siganus
12.20 12.00	nanostructured gradient index	fuscescens (Houttuyn, 1782) in the
	component and its developments	coastal of Quang Binh, Vietnam
	O-01	O-07
	Thi Hong Quan Vu	Thi Hoang Ha Truong
	Investigation of spectroscopic properties of Ba <sub>2</sub> MgMoO <sub>6</sub> double	Effects of mulch C/N ratio and de- composition stage on plant N uptake
12:30-12:40	perovskite doped with Eu <sup>3+</sup>	and N availability in soil with or
	ρετονεκίτε αορέα with Lu	without wheat straw incorporation
	O-02	O-08
	Hong Hanh Cong	Thanh Le Hai
	Green synthesis silver	Sustainable promotion of cultural
12:40-12:50	nanoparticles using Syzygium	landscape values in the Son river
	nervosum aqueous leaf extract	basin, Quang Binh, Vietnam
	O-03	O-09
	Thi Thu Ha Nguyen	Yen Tran Thi
	Ab-initio study of the magnetic	Research on the reproductive
12.50 12.00	properties of the double perovskites	characteristics of the blood cockle
12:50-13:00	$A_2MM'O_6$ compounds, where $A =$ alkaline earth or rare-earth metal	(Anadara granosa) in the coastal areas of Quang Binh province
	and M, M' = transition metals	areas of Quang Bum province
	<b>O-04</b>	O-10
		0.10
13:00-14:00	Lunch break	
	Session 3A Natural Science-2	Session 3B Biology
	Lecture hall 110N	Lecture hall 111N
	Online meeting: Enter here	Online meeting: Enter here
	Chairman: Mai Suan Li	Chairman: Andrzej Kornaś
	Hung Son Nguyen	Agnieszka Czyżowska
14.00 14.20	Ethical AI	The role of lipid peroxidation in
14:00-14:30	<ul> <li>principles and difficulties</li> </ul>	skeletal muscle atrophy and weakness
	I-3	in aging <b>I-5</b>
	Thang Do	Barbara Dyba
14:30-14:40	New study on the age of tertiary	Specific methods for studying the
	sediments in the Yen Bai basin	interaction between cell membrane
	(Northern Vietnam) based on	and environment under stressful
	palynological analysis	conditions
	O-05	0-11
14.40 14.50	NT.H. Kim-Ngan	Magdalena Skórka
14:40-14:50	MeV ion-beam for analysis and	Evaluation of manganese as a stress
	modifications of materials: the	factor in plant cells

	crystallinity and stability of the Fe <sub>3</sub> O <sub>4</sub> -based thin films O-06 e-Posters-1 online 3 min3 slide presentation	O-12 e-Posters-2 online 3 min3 slide presentation
14:50-15:20	P-01, P-02, P-03, P-04, P-05, P-06, P-07, P-08.	P-09, P-10, P-11, P-12, P-13, P-14, P-15, P-16.
	Sunday, November 2	1, 2021
	Lecture   Online meetin Chairman:	Biophysics hall 110N ag: Enter here Mai Suan Li
10:00-10:45	SARS-CoV-2 a a deadly journey from genes <b>Pl</b>	A Anh Tuan and COVID-19: mutations to cytokine storms 2-2
10:45-10:50	5 minut  Session 5A Biophysics and Physics	es break Session 5B Physics
	Lecture hall 110N  Online meeting: Enter here Chairman: Mai Suan Li	Lecture hall 111N  Online meeting: Enter here Chairman: Tran Quoc Tien
10:50-11:20	Trinh Xuan Hoang Protein escape at the ribosomal exit tunnel: insights from simple models I-6	Artur Błachowski Mössbauer studies of iron-based superconductors I-8
11:20-11:30	Hung Nguyen Electrostatic interactions explain the higher binding affinity of the CR3022 antibody for SARS-CoV-2 than the 4A8 antibody	Van Long Le Temperature dependence of anisotropic dielectric tensor of single-crystal α-SnS
	O-13 Mattia Longobucco	O-17 Jacek Gatlik
11:30-11:40	Study of all-optical switching of 1560 nm femtosecond pulses using soft glass dual-core fibers	The mass problem in effective description of soliton motion
	0-14	O-18
10:40-11:50	Sylwia Sowa Superconductivity and structure of selected 5f and (3-5)d metals and their hydrides	e-Posters-3 (10:35-10:50) online 3 min3 slide presentation P-17, P-18, P-19, P-20.
	O-15	1 17,1 10,1-17,1-20.
11:50-12:10	Coffee/t	ea break
	Session 6A Science and life-1 Lecture hall 110N Online meeting: Enter here	Session 6B Science and life-2 Lecture hall 111N Online meeting: Enter here
	Chairman: Dawid Nalęcz	Chairman: Vo Van Thiep

	Phan Anh Tu	Zbigniew Tarnawski
	Sustainable development for the	Diet guideline, is it an evidence -
12:10-12:40	Khmer community in Mekong delta	based science or food industry
12.10 12.10	(Vietnam) in the globalization context	advertisement?
	I-7	I-9
	Nguyen Phuong Nhung	Anna Kocoń
	A protein network for the	A review of ticks in Cracow,
12.40.12.50	prioritization of telomere interacting	Poland's most popular tourist city
12:40-12:50	oncogenes associated with non-small	
	cell lung cancer	
	O-16	O-19
	e-Posters-4	Sylwia Koczanowicz
	online 3 min3 slide presentation	The risk of tick attacks Ixodes ricinus
12:50-13:00		(Linnaeus, 1758) on selected tourist
12.30-13.00	P-21, P-22.	trails and educational-environmental
		paths in the Poprad landscape park
		O-20
13:00-13:05	5 minute	es break
	Special session: The first and	
		g: Enter here
	Chairmen: Tran Anh	Tuan, Le Xuan Lam
	Mai St	
13:05-13:15	Awarding the prize of Vietnam Asso	
	in Poland for the Young Scienti	
		years 2016-2021.
13:15-13:25	Presentation of the first laureate: Summary of the achievements  SO-1	
	Presentation of the second laurea	
13:25-13:35	SC	• •
	Summary a	
13:35-13:45	Online meetin	
13.33 13.73	Chairmen: Mai Suan Li, Hoa	
	Andrzej	
	Summary (N	
	Statistics (Kim N	<u> </u>
	Closing (And	irzej Kornas)
13:45-14:30	On-line round-t	table discussion

PL - Plenary lecture

O - Oral talk

SO - Special oral talk

I - Invited talk

P - Poster

	e-Posters		
		online 3 minute-3 slide presentation	
Poster	Presenting	Title	
	author		
P-01	Quan Dau	The fixed point theorem in a banach space Endowed with a digraph	
P-02	Thi Ly Mai	First-principle study of electronic properties of superconducting $\beta$ - $IrSn_A$	
P-03	Nguyen Ngoc Anh	Synthesis and characterization of thermal conductivity of nanofluids based on Ag decoreated CNTs-graphene hybrid materials	
P-04	Nguyen Thi Mai	Size-dependent geometric, electronic and $H_2$ adsorption properties of $Ag_nCr$ (n=1-12) clusters	
P-05	Manh Xuan Vu	Real-time, continuous-flow determination of the magnetic nanoparticles concentration by modified-GMR sensor	
P-06	Hoang Thien Ly	Sickest-first policy and predictive models for liver transplant candidates in the US	
P-07	Nguyen Thi Bich Lien	Design a website for looking up diplomas and certificates on the website qbu.edu.vn	
P-08	Cong Ngoc Phan	Change in electrical conductivity of river water due to the impact of small-scale hydroelectric system. Case study: Nida river, Poland	
P-09	Le Dang Huy	Combined ligand-based and structure-based virtual screening approach and molecular dynamics simulation of SARS-CoV-2 protease (Mpro and PLpro) for identifying antiviral inhibitors against SARS-CoV-2	
P-10	Le-Quang Bao	A simple rule-based approach for designing novel dual-target AChE and BACE1 inhibitors as anti-Alzheimer agents	
P-11	Le Khanh Vu		
P-12			
P-13	Phan Nu Y Anh	Factors affecting ecotourism development of Hac Hai lagoon, Quang Binh province	
P-14			
P-15	Nhung Hoang Thi Tuyet		
P-16	Ngan Nguyen Hoang	Evaluation of regulating effect on exogenous dyslipidemia of capsules prepared from fermented Allium sativum, Hibiscus sabdariffa, Gynostemma pentaphyllum and Alisma plantago aquatica on white rats	
P-17	Bui Thi Hoa	Transition metal (Co, Ni, Fe)-based materials -superior electrocatalyst for water splitting	
P-18	Ke Son Phan	Co-loading of nanosilver and nanoemulsion antibiotics plant- based Allium sativum extract in alginate/carboxyl methylcellulose carrier for antibacterial activity	

P-19	Le Thi	Degradation of methyl blue by an approach using plasma jet
	Quynh Xuan	processing
P-20	Michał	Locally anisotropic field in polydispersed composites after FSP
	Stawiarz	modification
P-21	Hoang	Administrative reform below the Minh Menh dynasty (1820 - 1840)
	Phuong Thao	
P-22	Joanna	Indo-Himalayan protected areas: mountain tourism
	Mostowska	

The program of WVSP2021 and PolVietSym2021 is based on plenary lectures (45 min.), invited talks (30 min.), contributed talks (10 min.) and poster presentations (each as (online) 3 minute-3 slide presentation (e-poster)).

Chương trình của WVSP2021 và PolVietSym2021 bao gồm các báo cáo tổng quan (thời lượng 45 phút), các báo cáo của khách mời (30 phút), các báo cáo đóng góp (10 phút) cùng với các báo cáo dạng poster (mỗi báo cáo được trình bày theo dạng 3-trang-trong-3-phút (e-poster)).

Program WVSP2021 i PolVietSym2021 opierają się na wykładach plenarnych (45 min.), wystąpieniach zaproszonych (30 min.), prezentacji ustnych (10 min.) oraz prezentacji plakatowych (każda jako 3 minut-3 slajdy-prezentacja (e-poster)).

#### Krakow time to several places' time conversion in November 2021

Oklahoma, USA -6	Kraków (CET)	Petersburg, Russia +2	Novocherkassk, Russia +2	VietNam (ICT) +6	Adelaide, Australia +9:30
4:00	10:00	12:00	12:00	16:00	19:30
8:00	14:00	16:00	16:00	20:00	23:30

Plenary lectures and invited talks

## Hydrogen storage in metal hydrides – fundamental principles meet practical life

#### Ladislav Havela

Faculty of Mathemtics and Physics, Charles University, Prague

There is now an extended evidence that climatic changes, the global warming, is related to extended use of hydrocarbons, producing lot of CO<sub>2</sub>. One possible leeways is a switch to hydrogen economy, which does not need carbon. This brings considerable challenges to materials research, which come from interaction of construction materials with hydrogen gas.

The other major issue is a storage of H gas. Besides rather inefficient storing H in high pressure tanks or in a liquid form, the most sophisticated technique is to store H in compounds, from which it can be released e.g. by moderate heating. The positive feature, a very high volumetric density, exceeding that of liquid hydrogen, is compensated by relatively low stored H mass compared to the total mass of the hydride. Therefore an optimum solution for automotive applications has not been solved yet. Light materials as Mg do not exhibit sufficiently fast kinetics or need high temperatures to desorb H. Conventional material LaNi<sub>5</sub>, which can form hydrides up to LaNiH<sub>6</sub>, is relatively expensive and heavy, but is used is specific situations as ecofriendly medium. Very specific application is the storage of tritium at nuclear fusion devices in metallic uranium.

Seen from the point of view of fundamental research, hydrides represent an interesting probe into a metallic system. The most striking effect is volume expansion, which can reach tens of percent. For example, the volume difference between U and its hydride UH<sub>3</sub> is 60%. This gives us a tool opposite to hydrostatic pressure, which allows to probe the impact of bringing atoms closer together. The presence of H affects naturally also the bonding conditions. H as rather electronegative element tends usually to host rather more electrons than 1, and theoretically the 1s states can accommodate up to 2 electrons per atom. The product, negatively charged H<sup>-</sup>, can increase its size enormously (in extreme case the diameter expands by a factor of 3), as the number of electrons is doubled. A dramatic impact it has also on electropositive elements as lanthanides or actinides.

Lanthanides, the elements with open (unfilled) and very stable 4f shell responsible for magnetism should be inert with respect to hydrogenation, as atomic magnetic moments come from the 4f shell, which cannot be perturbed by H atoms nearby. However, just the opposite is true. Long-range ordering of the moments, be it ferro- or antiferromagnetic, needs conduction electrons to mediate the spin interaction between individual lanthanide atoms. Those electrons (5d, 6s) are affected by the H bonding and they are literally filling the empty H-1s states. Hence they are not available for electrical conduction or for service as interaction moderators. This shows up in a dramatic decrease or ordering temperatures, below which a material becomes magnetically ordered. e.g. the Curie temperature  $T_{\rm C} = 297$  K in Gd metal drops by two orders of magnitude in GdH<sub>3</sub> (antiferromagnet with the Néel temperature  $T_{\rm N}$ 

determined as 3.32 K, while  $GdH_2$  has  $T_N = 21$  K. This phenomenon is another manifestation of the switchable mirror effect [1], based on the reversible loss of metallicity between  $YH_2$  and  $YH_3$ .  $YH_2$  is still metallic and gives mirror reflections, non-metallic  $YH_3$  is transparent. H absorption, which takes few seconds in a thin film, can swich therefore easily between reflecting and non-reflecting case.

It is interesting that in actinides, the 5f analogues of lanthanides, the same mechanism has entirely opposite impact on magnetism. The difference stems from the fact that the 5f states have a larger spatial extent within an atom. Therefore they overlap between neighbours and do not need any intermediary to convey the spin information. The volume expansion promotes larger magnetic moments on e.g. uranium, as the electron correlations forming the atomic moments (and yielding the Hund's rules) are not so much disturbed by the metallic bond, including in this case also the 5f states. In another words, the 5f band becomes narrower. But this is not whole story. The 6d states of U do not play in this situation the necessary interaction link, but they can hybridize with the 5f states and can reduce or suppressed the 5f magnetism. In the hydrides they couple to the H-1s states and the 5f states are free to form the moments. Consequently, U metal has a normal non-magnetic ground state. UH<sub>2</sub> is ferromagnet with  $T_C = 125$  K [2], UH<sub>3</sub> has  $T_C = 165$  K, and if the H/U ratio is modified by chemical substitutions  $T_C$  can exceed 200 K. In this case there is not loss of metallicitity, the 5f electrons remain in the conducting band.

Very special materials are so called polyhydrides, which can be viewed as metallic hydrogen, elusive material existing perhaps at extreme pressures, with isolated atoms of e.g. lanthanides or actinides, which contribute to bonding and bring thus the range of existence to still very high but achievable pressures in laboratories. Such substances are superconducting with very high critical temperatures (260 K in LaH<sub>10</sub> [3]), but they decompose if they are take away from a diamond anvil cell, where they were created at the hydrogen pressure of 190 GPa. However, there is still a hope that some of such substances may be stable and survive with hydrogen inside.

#### Acknowdlegment

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#### References

- [1] J.N. Huiberts, R. Griessen, J.H. Rector, R.J. Wijngaarden, J.P. Dekker, D.G. de Groot, and N.J. Koeman, Nature 380 (1996) 231.
- [2] L. Havela, M. Paukov, M. Dopita, L. Horak, D. Drozdenko, M. Divis, I. Turek, D. Legut, L. Kyvala, T. Gouder, A. Seibert, F. Huber, Inorg. Chem. 57 (2018) 14727.
- [3] M. Somayazulu, M. Ahart, A.K. Mishra, Z.M. Geballe, M. Baldini, Y. Meng, V.V. Struzhkin, and R.J. Hemley, Phys.Rev.Letters 122 (2019) 027001.

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## SARS-CoV-2 and COVID-19: a deadly journey from genes mutations to cytokine storms

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The SARS-CoV-2, which is responsible for the current Coronavirus disease (COVID-19), has currently affected >200 countries. As of September 19, 2021, about 230 million people have been infected, with more than 4.6 million deaths [1]. More than 5.8 billion people have been vaccinated, but many infected people end up in critical conditions that require respiratory assistance [2].

Although SARS-CoV-2 can theoretically infect various organs after binding to the ubiquitous ACE-2 cell membrane receptor, the respiratory system is practically the most frequently impacted due to the airborne nature of the infective agent [3]. Although the clinical picture is very heterogeneous, the potential for severe lifethreatening conditions in adults comes from the respiratory component of the disease: airways, alveolar and vascular damage, inflammation, dysfunction, and repair can lead to rapidly progressive acute hypoxemic respiratory failure [4]. Since its appearance in December 2019, it has become rapidly obvious that this new disease behaves very differently from previously known viral pneumonias in terms of risk factors, biological, radiological, and clinical presentation, natural course and response to therapy, making specific research and clinical guidance mandatory to understand the disease, deliver appropriate care and support public health decisions.

Adaptive mutations in the SARS-CoV-2 genome could alter its pathogenic potential, and at the same time would increase the difficulty of drug and vaccine development. Generally, the rates of nucleotide substitution of RNA viruses are fast, and this rapid evolution is mainly shaped by natural selection. This high error rate and the consequent rapidly evolving virus populations, which could lead to the accumulation of amino acid mutations, might affect the transmissibility of the virus, its cell tropism and pathogenicity. Based on the recent epidemiological update by the WHO, as of September 19, 2021, four SARS-CoV-2 VOCs have been identified since the beginning of the pandemic:

- Alpha (B.1.1.7): first variant of concern described in the United Kingdom (UK) in late December 2020
- Beta (B.1.351): first reported in South Africa in December 2020
- Gamma (P.1): first reported in Brazil in early January 2021
- **Delta (B.1.617.2):** first reported in India in December 2020

Despite the extraordinary speed of vaccine development against COVID-19 and continued mass vaccination efforts across the world, the emergence of these new variant strains of SARS-CoV-2 threatens to overturn the significant progress made so far in halting the spread of SARS-CoV-2.

By September 2021, we can state that much has been learned about the pathogenesis, epidemiology, and clinical management of COVID-19 since its outbreak

in December 2019. We are not aware of any other medical condition that would have ever had such a "high speed" dynamic in the emergence of medical knowledge, as reflected in the unprecedented exponential rise in scientific publications during the past 20 months. Despite all the imperfections in the system and the hardship and suffering the pandemic has caused, COVID-19 has also shown how creative and productive humans can be if they work together. Unfortunately, we must expect that COVID-19 will persist as a major challenge for the delivery of medical care for a long while to go, and nothing is fast enough when it is about survival of an individual or a society.

#### References

- [1] Johns Hopkins Coronavirus Resource Center https://coronavirus.jhu.edu/map.html
- [2] Pollard CA, Morran MP, Nestor-Kalinoski AL. The COVID-19 pandemic: a global health crisis. *Physiol Genomics*. 2020 Nov 1;52(11):549-557.
- [3] Salian VS, Wright JA, Vedell PT, Nair S, Li C, Kandimalla M, Tang X, Carmona Porquera EM, Kalari KR, Kandimalla KK. COVID-19 Transmission, current treatment, and future therapeutic strategies. *Mol Pharm*. 2021 Mar 1;18(3):754-771.
- [4] Berlin DA, Gulick RM, Martinez FJ.Severe Covid-19. *N Engl J Med*. 2020 Dec 17;383(25):2451-2460.
- [5] European Centre for Disease Prevention and Control. https://www.ecdc.europa.eu/en/covid-19/variants-concern

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### The values in Vietnamese Mother Worship

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Spiritual culture, holy culture has been always an essential aspect in every society, every phase of social development. This is one of the elements that anchor the soul and humanity as well as form cultural identity of each culture.

What mentioned in this article is the Mother Worship - a very special socio-cultural phenomenon in Vietnam. The Mother Worship has a long and profound history with a durable position in Vietnamese spiritual life. This article introduces and analyses three factors of Vietnamese Mother Worship: the origin, development process and its values. First of all, its formation originates from the general context of the formation of primitive religions and beliefs of mankind; indigenous polytheism of Vietnamese people and the matriarchy of the inhabitants in the culture based on wet rice farming. Secondly, the development process starts from Goddess worship generally speaking, Mother Worship, "Tam Phu" and "Tu Phap" Worship in the North Vietnam to the Queen/Mother of land in the Central and South Vietnam. Thirdly, expressions and values of Mother Worship are so diverse. Mother Worship can embody or mean a deity that is enshrined in each village's communal temple, symbolize gender equality, the Mom to care, protect, tolerate, nurture people and things, help people orientate toward goodness and unite community cohesion.

In order to gain above-mentioned purposes, the article applies comparative cultural studies specifically Affectual/Consequential comparison, Synchronic and Diachronic comparison, feminism perspective and analytic-synthetic method.

The findings of the article discloses some similarities and differences in Mother Worship in three regions in Vietnam. Thus, it will help the audience have better understanding and knowledge of a beautiful custom of Vietnamese people.

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# 1/f noise characterization of MgO-based magnetoresistive sensors enable a noise-based technique for detecting of weak magnetic signals

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Magnetoresistive (MR) sensors are linear magnetic field transducers based either on the intrinsic magnetoresistance of the ferromagnetic (FM) material (anisotropic magnetoresistance (AMR) sensors) or on FM/nonmagnetic heterostructures (giant magnetoresistance (GMR) multilayers, spin valve (SV), tunneling and magnetoresistance (TMR) devices) in which the resistance of the sensor depends on the relative orientation of the magnetization of FM layers. Among these MR sensors, magnetic tunnel junction (MTJ) based TMR sensors are considered promising candidates for the detection of magnetic nanoparticles (MNPs) as biomarkers and the biomagnetic fields due to their high MR ratios and high field sensitivities to detect small changes in magnetic fields [1]. However, noise problem, specially 1/f noise which is often quite large at low frequencies, limits the sensitivity of MTJ sensors for ultra-low magnetic field applications [2,3]. The presence of magnetic domains in the active region of the sensor which is known as the main source of 1/f noise in low frequency for MR sensors [4,5].

This talk is dedicated to the discussion of the state-of-the-art on MR sensors, and challenging for biosensor applications. We will give an introduction about TMR based sensors including: TMR elements, characterization of TMR thin films and devices, noise and the reduction of low frequency noise in TMR sensors as well as different MNPs detection strategies. In our work, to enhance the sensitivity and decrease 1/f magnetic noise, we proposed the use of deepmicron sized MTJs which are closed to the near-single or single magnetic domain state. In such nanoscale MTJs, due to the low or zero domain wall density the magnetic noise owing to domains and domain walls fluctuate is minimal [6]. By using this approach, we can decrease the measured noise level to values close to the minimum attainable thank to the reduction of the inhomogeneous fluctuations in the smaller deep micrometer-sized MTJs. The homemade low frequency noise setup and the use of noise measurement for detecting of weak magnetic signals are also discussed. The research suggests the new approach for a noise-based technique for detecting extremely weak magnetic fields generated by biological sources.

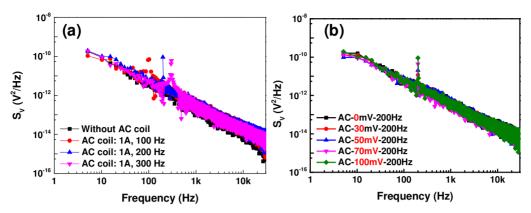


Figure 1. Noise spectral density  $S_V$  as a function of frequency for a 400 nm MTJs with and without a small AC field (various frequencies (a) and voltages(b)) showing that the small AC field is detectable.

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#### References

- [1] Z. Jin et al., AIP Advances 11 (2021) 015046
- [2] W.F. Egelhoff Jr et al., Sensors and Actuators A 155 (2009) 217–225
- [3] Z.Q. Lei et al., IEEE Trans. Magn. 47 (2011) 602-612
- [4] C. Fermon et al., Sens. Actuators A 129 (2006) 203–206
- [5] A.F.M. Nor et al., IEEE Trans. Magn. 34 (1998) 1327–1329
- [6] A. Nguyen, et al., Appl. Phys. Lett. 129 (2021) 024503

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### **Ethical AI – principles and difficulties**

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Artificial intelligence (AI) is a wide-ranging tool that enables people to rethink how we integrate information, analyze data, and use the resulting insights to improve decision making, and already it is transforming every walk of life.

Artificial intelligence can improve people's decision-making, but it has its limitations. It is possible that the bias of the algorithms may create ethical risks that call into question the reliability of the data generated by the system. The deviation can be explained by explaining the data, reproducibility in testing for consistent results, and controllability. Other ethical threats include lack of transparency, erosion of privacy, weak accountability, and the movement and transition of workers. The existence of such a risk affects whether to trust AI systems. To build trust through transparency, organizations should clearly explain what data they collect, how it is used, and how the results affect customers.

Ethics is important, both in our personal and professional lives. Standards such as honesty, integrity, honesty, accountability and accountability, along with transparency, underlie ethical artificial intelligence (AI) systems. Ethical AI is the foundation on which you build trust in your system. About a third of executives in a Deloitte survey cited ethical risk as one of the top three concerns with AI.

According to Vincent Müller in his book [1], AI ethics is a branch of technological ethics specific to AI systems. Sometimes it is broken down into concern for the moral behavior of the people who design, manufacture, use and treat artificially intelligent systems, and concern for the behavior of machines or the ethics of machines.

In this talk, we will study the principles that govern the ethical use of artificial intelligence. We will analyse the five guiding pillars of ethics in artificial intelligence proposed by Todd Lohr and Traci Gusher from KPMG <sup>1</sup>:

**Transforming the workplace:** The massive shift in the roles and tasks that define work, along with the development of powerful analytical and automated decision making, will result in a shift in work and the need for retraining.

**Establish governance and governance:** The new rules will set guidelines for the ethical use of AI and protect the well-being of society.

**Aligning cybersecurity and ethical AI:** Autonomous algorithms cause cybersecurity threats and enemy attacks that can contaminate algorithms by manipulating data. In 2019, 72 percent of U.S. CEOs agree that strong cybersecurity is critical to instilling the trust of their key stakeholders, up from 15 percent in 2018.

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<sup>&</sup>lt;sup>1</sup> http://advisory.kpmg.us/

**Bias Mitigation:** Understanding how sophisticated, autonomous algorithms work is essential to taking steps to eliminate unfair biases as they evolve.

**Increased Transparency:** Universal standards of integrity and trust should guide general governance principles for the ethical use of AI.

We also discuss the difficulties in implementing the above principles. According to Xuhui Shao, managing partner of Los Altos, Calif.-based Tsingyuan Ventures "A new class of general purpose adversarial neural networks can be built to examine and discriminate against other AI systems to produce human-understood interpretations and to check for hidden biases or flaws," he said. "As more consumers and businesses become aware of the importance of ethical AI, these types of safeguards will become more prevalent by 2030." <sup>2</sup>

#### Reference

[1] V. C. Müller, Ethics of Artificial Intelligence and Robotics, in: E.N. Zalta (Ed.) ,The Stanford Encyclopedia of Philosophy, Summer 2021 ed., Metaphysics Research Lab, Stanford University, 2021.

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 $<sup>^2\,\</sup>underline{\text{https://www.reworked.co/information-management/why-ethical-ai-wont-catch-on-anytime-soon/}}$ 

# The power of plants – application of fossil spores and pollen grains in geology

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To ensure the survival of species, plants, being sedentary organisms, have to disperse their genetic material *via* wind, water or animals. To protect the material during transportation plants produce special capsules extremely resistant to external conditions. They are called spores and pollen grains. Their wall is made of sporopollenin – one of the most stable biological polymers. It causes they are frequent fossils in many kinds of clastic rocks. Fossilised spores and pollen grains are called palynomorphs.

To make a release of cytoplasmic content of spores and pollen grains possible, some parts of their wall remains thinner. In pollen grains these thinner parts are named apertures and take a form of pores or furrows. The outer layer of spores and pollen grains is usually sculptured. The combination of grain's shape, sculpture and type of apertures allows to determine plants that have produced a given type of palynomorphs. And this possibility remains a crucial feature in geology. When reconstructing history of the Earth geologists need to know the age of sediments. Very useful are here fossils. In sediments deposited in terrestrial conditions animal fossils are rather rare but, on the contrary, palynomorphs are frequently encountered. When parent plant taxa are already indicated it is possible to reconstruct plant assemblages that occupied a region during deposition of the sediment. And this, by comparison with other known past plant assemblages, allows to determine age of the rocks. Not only the age can be reconstructed but also environmental conditions under which plants thrived, as well as paleoclimate. Obviously lots of doubts and questions occur during both palynological analysis and age, environmental and climatic interpretations. However, fossil spores and pollen grains remain a powerful tool in geological practice.

A good examples of palynological studies are papers by Wysocka et al. (2018, 2020) [1,2]. They concern material from Northern Vietnam. Fossil palynomorphs allowed authors to say that sediments studied were deposited close to the Eocene/Oligocene transition. Also an existence of riparian and mixed-mesophytic forests in the vicinity of the depositional basin was indicated and a climate was shown to be warm-temperate to subtropical.

#### References

- [1] Wysocka A., Pha D.P., Durska E., Czarniecka U., Thang D.V., Filipek A., Cuong N.Q., Tuan D.M., Huyen N.X. and Tha H.V. (2018). New data on the continental deposits from the Cao Bang Basin (Cao Bang-Tien Yen Fault Zone, NE Vietnam)-biostratigraphy, provenance and facies pattern. Acta Geologica Polonica, 68 (4), 689-709.
- [2] Wysocka A., Pha D.P., Durska E., Czarniecka U., Thang D.V., Filipek A., Cuong N.Q., Tuan D.M., Huyen N.X., Tha H.V., and Staniszewski R. (2020). The Na Duong Basin (North Vietnam): A key for understanding Paleogene basin evolution in relation to the left-lateral Cao Bang-Tien Yen Fault. Journal of Asian Earth Sciences, 195.

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# The role of lipid peroxidation in skeletal muscle atrophy and weakness in aging

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The pathological age-related loss of skeletal muscle mass and strength (sarcopenia) contributes to decreased quality of life and increases the risk of injury and chronic disease. The causes of sarcopenia are still unknown, but it is known that the generation of reactive oxygen species is a characteristic for aging muscles [1]. Oxidative stress leads, among other things, to the initiation of a chain reaction of lipid peroxidation.

The main aim of the study was to determine the role of lipid peroxidation in sarcopenia. Particular attention was paid to the role of lipid hydroperoxides (LOOH), lipid signaling molecules (oxilipins), and enzymes involved in the pathways of oxidized lipid metabolism.

Lipid hydroperoxides (LOOH) generated by iron-mediated lipid oxidation lead to cell death known as ferroptosis [2]. The mechanisms involved in cell death due to the high LOOH load and the role of ferroptosis in age-related loss of muscle mass and function remain unclear. Phospholipid hydroperoxide glutathione peroxidase (Gpx4) is considered the main regulator of ferroptosis due to its ability to directly reduce peroxidized phospholipids and other hydroperoxides that have been produced in cell membranes [3]; therefore its activity and role in sarcopenia prevention is the main goal of the presented research. Oxylipins, which are oxygenated derivatives of polyunsaturated fatty acids (PUFAs) formed enzymatically either by lipoxygenases (LOX) or cyclooxygenase (COX), are another important cellular component in aging muscle. Metabolites formed from archaidic acid (AA) and linoleic acid (LA) as a result of 12/15-LOX activity seem to be of particular importance. The enzymes that increase the amount of AA in cells by its release from membrane lipids are phospholipases A2 (PLA2). These enzymes can be a key target in preventing the death of muscle cells as a result of ferroptosis.

The presented studies indicate that ferroptosis may play an important role in agerelated loss in muscle mass and function, paving the way for further research and contributing to the development of new targeted therapies.

#### References

- [1] S. Mankhong, S. Kim, S. Moon, H.B. Kwak, D.H. Park, & J.H. Kang. Experimental models of sarcopenia: bridging molecular mechanism and therapeutic strategy. Cells. (2020) 9(6), 1385.
- [2] J. Li, F. Cao, H.L.Yin, Z.J. Huang, Z.T. Lin, N. Mao, ... & G. Wang. Ferroptosis: past, present and future. Cell death & disease. (2020) 11(2), 1-13.
- [3] J.P.F. Angeli, M. Schneider, B. Proneth, Y.Y. Tyurina, V.A. Tyurin, V.J. Hammond, ... & M. Conrad. Inactivation of the ferroptosis regulator Gpx4 triggers acute renal failure in mice. Nature cell biology. (2014) 16(12), 1180-1191.

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# Protein escape at the ribosomal exit tunnel: insights from simple models

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In cells, proteins are synthesized by the ribosome which translates the genetic information carried by mRNA. During synthesis, amino acids are polymerized at the peptidyl transferase center (PTC) onto a growing nascent chain, which must traverse through a tunnel before emerging from the ribosome. This tunnel, namely the ribosomal exit tunnel, is a narrow passage of ~80-100 Å in length and ~10-20 Å in diameter located in the large ribosomal subunit. Such passage helps to protect nascent chains from aggregation and is known to be involved in the regulations of translation and nascent protein folding. While there are many studies on co-translational protein folding, i.e. the folding during protein synthesis, few studies have focused on post-translational processes, such as the escape of a full-length protein from the ribosome tunnel. The latter process is important as a too quick escape would make a partially folded protein vulnerable to aggregation whereas a too slow escape or a kinetically trapped protein could jam the ribosome tunnel.

In this talk, I will discuss how newly synthesized proteins escape from the ribosomal exit tunnel with the help of coarse-grained molecular dynamics simulations and a simple diffusion model based on the Smoluchowski equation. There will be relevant issues such as the coupling between the folding and the escape process, the role of the size and shape of the tunnel and the effects of energetic interactions between nascent proteins and the ribosome tunnel. Our studies [1-4] suggest that the length of the ribosomal exit tunnel has been chosen by evolution to facilitate both the efficient escape and the correct folding of nascent proteins. Folding and escape are concomitant and enhance each other. The estimated escape times are found in the sub-millisecond to millisecond timescale, indicating that the escape does not delay the ribosome recycling. The remarkable agreement of the escape time distribution with the diffusion model suggests that the escape process is simple and predictable. It seems that such characteristics are necessary for the efficient folding of nascent proteins and for the smooth functioning of ribosomes.

#### References

- [1] P. T. Bui and T. X. Hoang. Folding and escape of nascent proteins at ribosomal exit tunnel. J. Chem. Phys. 144, 095102 (2016).
- [2] P. T. Bui and T. X. Hoang. *Protein escape at the ribosomal exit tunnel: Effects of native interactions, tunnel length, and macromolecular crowding.* J. Chem. Phys. 149, 045102 (2018).
- [3] P. T. Bui and T. X. Hoang. *Protein escape at the ribosomal exit tunnel: Effect of the tunnel shape.* J. Chem. Phys. 153, 045105 (2020).
- [4] P. T. Bui and T. X. Hoang. *Hydrophobic and electrostatic interactions modulate protein escape at the ribosomal exit tunnel*. Biophys. J. 120, in press (2021).

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# Sustainable development for the Khmer community in Mekong delta (Vietnam) in the globalization context

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Ethnic minority groups in Vietnam have suffered a tremendous impact as a result of globalization. Globalization and regionalization processes have had a direct impact on the Mekong Delta region in the current setting. As a result of this consequence, the conventional perspective of indigenous groups has shifted, because these groups founded their economies and cultural lives on traditional agricultural systems. The Khmer is one of the four major ethnic groups that have had a long residence history in the Mekong Delta, including the Khmer, the Viet (Kinh group), the Chinese Vietnamese and the Cham. With their distinctive traditional cultural characteristics, the Khmer people have been mainly residing in villages far away from the urban. Globalization and climate change have had direct impacts on the Khmer's livelihoods and culture. Nowadays, an increasing number of the Khmer have left their rural areas to migrate to big cities in Southern Vietnam. The traditional culture of Khmer people has been transformed and the organizational structure of traditional Khmer society in South Vietnam has been compromised under the impact of the process of labor migration and their shifting lifestyle.

The purpose of this article is to demonstrate the direction of sustainable development for the Khmer community in the Mekong Delta by evaluating the Vietnamese government's policies on ethnic groups, culture preservation, and living environment for indigenous peoples under the effect of globalization. The research result will contribute to the sustainable development platform for the Khmer community in Southern Vietnam.

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### Mössbauer studies of iron-based superconductors

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Mössbauer spectroscopy is a technique used to study nuclear structure with the absorption and re-emission of gamma rays. In its most common form, Mössbauer absorption spectroscopy, a solid sample is exposed to a beam of gamma radiation, and a detector measures the intensity of the beam transmitted through the sample. The atoms in the source emitting the gamma rays must be of the same isotope as the atoms in the sample absorbing them. We have used the Mössbauer spectroscopy of the 14.41 keV line of the iron isotope <sup>57</sup>Fe. The measurements can be performed in the temperature range from 1.5 K to 1100 K and in a magnetic field up to 7.5 T (Fig. 1). One of the research topics is the superconductivity in the iron-based compounds.



Figure 1. Mössbauer Spectroscopy Laboratory, Institute of Physics, Pedagogical University of Cracow.

Iron-based superconductors (FeSC) belong to compounds of iron pnictides and iron chalcogenides with layered tetragonal structure. The superconducting properties were first discovered in 2006 in LaOFeP [1]. In 2008, it was showed that the iron pnictide LaOFeAs(F,O) undergoes superconducting transition at the critical temperature  $T_{\rm sc}=26~{\rm K}$  [2]. Since then several families of superconductors based on Fe-As or Fe-Se layers was found (Fig. 2). Due to their relatively high critical temperature, high upper critical field and small anisotropy, iron based superconductors have attracted a large attention with respect to technical application, particularly at low temperature and high fields.

In this work, iron-based superconductors with different type of doping, i.e.  $Ba_{1-x}K_xFe_2As_2$  (hole-doping),  $SmFeAsO_{1-x}F_x$  (electron-doping), and  $BaFe_2(As_{1-x}P_x)_2$  (isovalent-substitution) [3], were investigated by means of  $^{57}Fe$  Mössbauer

spectroscopy. Spectra were collected versus temperature with special attention paid to the region of superconducting transition, i.e. the critical temperature  $T_{sc}$ . Mössbauer spectra display quasi-continuous distribution of quadrupole doublets in the whole temperature range. A distribution is caused by the spatial modulation of the electric field gradient (EFG) being a consequence of the incommensurate modulation of the electron charge density at the Fe nuclei, i.e. the charge density wave (CDW). It was found that charge modulations strongly vary at critical temperature due to the superconducting gap opening and subsequent formation of the Cooper pairs.

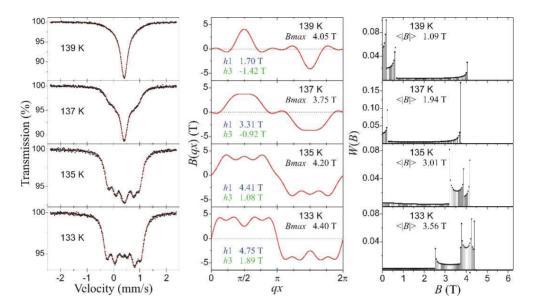


Figure 2. <sup>57</sup>Fe Mössbauer spectra of BaFe<sub>2</sub>As<sub>2</sub> parent compound within the temperature range of SDW magnetic order, the shape of SDW, and the magnetic field distribution.

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#### References

- [1] Y. Kamihara, H. Hiramatsu, M. Hirano, R. Kawamura, H. Yanagi, T. Kamiya, H. Hosono, J. Am. Chem. Soc. 128, 10012 (2006).
- [2] Y. Kamihara, T. Watanabe, M. Hirano, H. Hosono, J. Am. Chem. Soc. 130, 3296 (2008).
- [3] K. Komędera, J. Gatlik, A. Błachowski, J. Żukrowski, T.J. Sato, D. Legut, and U.D. Wdowik, Phys. Rev. B 103, 024526 (2021).

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## Diet guideline, is it an evidence-based science or food industry advertisement?

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It seems, that human kind is the only species on Earth, who does not know what should be the proper food. One point is clear; several chronic illnesses, which was very rare about 100 years ago, have become the main cause of shortening our active life and life itself nowadays. It poses a question, what has changed in the environment and our life-style, that brings us to the situation, that only a modest number (~12%) of the population is metabolically healthy. It is shown and argued, that the evolution let the human get an ability to survive in harsh and often scare of food environment. With such the ability of high adaptation, we have survived two millions years to become homo sapiens.

Until the 50s and 60s of the 20<sup>th</sup> century, we have ate mostly simple products of the Nature. Besides, we have had mainly three courses of home prepared food, without any snacks and/or sweets between meals. There were only seasonal fruits and vegetables, not whole year long. During the last 50-60 years, there is a rapid and continuous increase in number of cvd (cardiovascular), cancer, mental deterioration and other chronic illnesses. What is the reason? What is the correlation between the changes in our environment, our life-style and our health?

From the epidemiological studies (correlation and not cause-effect science), one should be able to get some understanding and form hypothesis, to be investigated experimentally. Dietary guidelines however are based mostly on epidemiological studies [1-3]. Such studies collects information, which now can be called "big data", which may be interpreted in many ways. Interpretation and conclusions are often biased by personal opinion or the opinion of one who sponsored.

What regards the food, since end of 19<sup>th</sup> century until the first part of 20<sup>th</sup> century, gradually increased consumption of sugar and the consumption of industry-produced and also hardened seed oils, promoted as modern and better fat. In other words, it was the moment in our history, when the food production became food industry, with its huge scale of production (and a huge money involved, as well as its benefit). It was not a problem to produce any amount of margarine or seed oils, or sugar, or all things, which we call now, a processed food. It was a question, how to make everybody use and eat them. The current status of our health, and the shelfs of our shops, are the evidence, how huge is the success in promoting processed food. First time in history, government advised what to eat, and formulated Dietary Goals, recommending that people avoid becoming obese by consuming only as much energy as was expended and to reverse obesity by decreasing energy intake and increasing energy expenditure. The Dietary Guidelines has been published every five years beginning in 1980, producing nine guidelines to date. One consistent recommendation of these nine guidelines has been that people reduce their dietary consumption of

saturated fat and animal products, including meat, dairy and eggs, and to increase their dietary consumption of carbohydrates and plant foods, including fruits, vegetables and grains. As stated, food pyramids were constructed to explain and promote healthy diet and to provide nutritional advice for people who are healthy or who are at risk for chronic disease but do not currently have chronic disease. It does not mean, that this advice is proper for still increasing percentage of the overweight or obese. The advice we need, is advice how to bring back homeostasis – metabolic balance, proper weight, and how to stop development and reverse chronic diseases.

In this work, the alternative food pyramids, built on evidence based science, will be discussed, with the goal to maintain or bring back metabolic balance, proper body composition, to stop and reverse chronic diseases.

#### References

- [1] L.K. English at al. (21 co-authors). Evaluation of Dietary Patterns and All-Cause Mortality. A Systematic Review. JAMA Network. A recommendation of Dietary Guidelines Advisory Committee to US Dietary Guidelines Committee **4**(8) (2021), e2122277. doi:10.1001/jamanetworkopen.2021.22277
- [2] Scientific Report of the 2020 Dietary. Guidelines Advisory Committee: Advisory Report to the Secretary of Agriculture and the Secretary of Health and Human Services. U.S. Department of Agriculture, Agricultural Research Service, Washington, DC.
- [3] J.S. Volek et al. Alternative Dietary Patterns for Americans: Low-Carbohydrate Diets. Nutrients **13**(10) (2021) 3299. <a href="https://doi.org/10.3390/nu13103299">https://doi.org/10.3390/nu13103299</a>

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Oral talks

### Effective generation of optical vortex beams using flat-surface nanostructured gradient index component and its developments

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Optical vortex beams (OVBs), also known as helical light beams, are characterized by doughnut-shaped intensity profile and phase singularities associated with orbital angular momentums [1]. Due to those unique properties, OVBs have found numerous potentials in various research fields and applications, to name a few, superresolution microscopy (Nobel prize 2014); particle manipulations; optical communications; quantum information processing; micro-machining; and astrophysics [2]. However, current available approaches for OVB generation suffer from at least one of following limitations: complex configurations, low efficiency, large size, high-cost fabrication and low integration. Therefore, there have been high demand of effective generation and flexible control of OVBs.

Here we present on theoretical and experimental studies on a single nanostructured gradient index vortex phase mask (nVPM). The nVPM is composed of a designed array of nano-sized rods which were made of two glass types with low and high refractive indices [3]. The refractive index distribution of a mask was calculated using the effective medium theory (EMT) [4] and simulated annealing approach [5]. Accordingly with the EMT the binary nanorod structure, while discrete, will behave as a continuous effective medium with effective index distribution equal to spatial average of neighboring refractive indices.

A cost-effective modified stack-and-draw technique was utilized for nVPM development. This approach is commonly employed for photonic crystal fibers fabrication. The typical fabricated nVPMs have an outer diameter of 125  $\mu$ m with a central hexagonal structure diameter of 20  $\mu$ m. The operation principle of the nVPM is defined by its internal refractive index profile, not by its surface profile. As a result, it has completely flat surfaces which allows it to be easily integrated to other optical elements and fiber systems. In this way, the optical performance of nVPMs is unaffected by the refractive index of the surrounding media no matter in air or in water or in ethanol media [6].

We have reported fiber-based microprobes with integrated nVPM at the end as an alternative replacement of a bulky setup of disparate elements for OVB generation [7]. This allows easy manipulation of generated OVBs in three dimentional space. Very recently, we successfully developed a novel compact and robust all-fiber micro-optical system to generate high-quality focused optical vortices without the use of any additional external optical devices. Our system consists of two nanostructured gradient

index microoptical components, i.e. vortex phase masks (nVPM) and lens (nGRIN lens) integrated onto the optical fiber tip. The single mode fiber (SMF) is used to ensure high quality of light illuminating the nVPM. The generation of an OVB with topological charge l=1 is experimentally verified. These experimental results are supported by numerical simulations. In addition, both simulations and experiments confirm that the created OVB focuses at a distance of 350  $\mu$ m. Similarly to the fiber microprobe reported earlier [7], our new integrated micro-optical system can be used in different transparent external media without degradation of its optical performance.

#### References

- [1] L. Allen, M. W. Beijersbergen, R. J. C. Spreeuw, and J. P. Woerdman, "Orbital angular momentum of light and the transformation of Laguerre-Gaussian laser modes". Phys. Rev. A, **45**(11), 8185 (1992).
- [2] Y. Shen, X. Wang, Z. Xie, C. Min, X. Fu, Q. Liu, M. Gong, and X. Yuan, "Optical vortices 30 years on: OAM manipulation from topological charge to multiple singularities". Light Sci. Appl. 8(1), 1–29 (2019).
- [3] K. Switkowski, A. Anuszkiewicz, A. Filipkowski, D. Pysz, R. Stepien, W. Krolikowski, and R. Buczynski, "Formation of optical vortices with all-glass nanostructured gradient index masks". Opt. Express, **25**(25), 31443 (2017).
- [4] A. Sihvola, Electromagnetic Mixing Formulas and Applications (IET, 1999)
- [5] S. Kirkpatrick, C. D. Gelatt, and M. P. Vecchi, "Optimization by simulated annealing," Science (80-.). 220(4598), 671–680 (1983).
- [6] H. T. Nguyen, K. Switkowski, R. Kasztelanic, and A. Anuszkiewicz, "Optical characterization of single nanostructured gradient index vortex phase masks fabricated by the modified stack-and-draw technique". Opt. Commun. **463** (January), 125435 (2020).
- [7] H. T. Nguyen, K. Switkowski, A. Filipkowski, R. Kasztelanic, D. Pysz, H.V. Le, R. Stepien, W. Krolikowski, and R. Buczynski, "Fiber microprobe with integrated gradient index vortex mask". Opt. Commun., 477, 126345 (2020).

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# Investigation of spectroscopic properties of Ba<sub>2</sub>MgMoO<sub>6</sub> double perovskite doped with Eu<sup>3+</sup>

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In this study, an investigation of spectroscopic properties of  $Ba_2MgMoO_6$  (BMM) double perovskites doped with  $Eu^{3+}$  was present. All samples were successfully synthesized by the co-precipitation method for the first time. The crystal structure and the morphology of the samples were investigated by using the powder X-ray diffractions and the scanning electron microscope analysis. Since  $Eu^{3+}$  ions are located in  $Mg^{2+}$  sites  $(O_h)$  with an inversion centre, the unique emission spectra of  $Eu^{3+}$  were observed with the dominance of the magnetic dipole transition ( ${}^5D_0 \rightarrow {}^7F_1$ ). Besides, the asymmetry factor R, which presents the changes of the surroundings of  $Eu^{3+}$  in the lattice, exhibits an increase from 1.08 to 1.18 corresponding to the sample doped 0.5% and 7%, respectively. The color of emission and the quantum yield were investigated as a function of  $Eu^{3+}$  concentration. Moreover, the temperature-dependent emission of BMM: 5%  $Eu^{3+}$  was measured and the quenching temperature was found to be at 260 K. Interestingly, the emission of the host was very stable up to 800 K.

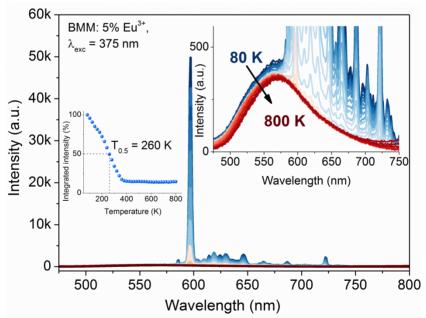


Figure 1. The temperature-dependent emission spectra of BMM: 5% Eu<sup>3+</sup> under 375 nm excitation from 80 K to 800 K

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# Green synthesis silver nanoparticles using *Syzygium nervosum* aqueous leaf extract

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Nowadays, finding alternatives to antibiotics is very urgent to reduce antibiotic resistance, which is a serious threat to human health. Silver is a natural antibacterial element, capable of killing a broad spectrum of pathogenic microorganisms. Simultaneously, silver, compared to the other metals, shows higher toxicity to microorganism, while it exhibits lower toxicity to mammalian cells [1]. Besides, synthesis methods of nanoparticles also contribute to its cost and toxicity for the environment [2]. The green synthesis method of nanoparticles has attracted wide attention because of its inherent features (simple, ecofriendly), which find its possible application in biomedical field specially in antimicrobial development [3, 4].

In this study, we used the extract of Syzygium nervosum leaves as a reducing agent to synthesize silver nanoparticles (AgNPs), which have been proven their antioxidant, anti-inflammatory, antiviral, and antibacterial activities [5-7]. The synthesized AgNPs were monitored by UV-Vis spectrophotometer and further characterized by dynamic laser scattering spectroscopy (DLS), field emission scanning electron microscopy method (FESEM). Effects of the ratio between the leaves extract and the used amount of AgNO<sub>3</sub>, as well as the stabilizers (Polyvinyl Alcohol, Polyvinylpyrrolidone, β-cyclodextrin, chitosan) on the formed AgNPs were also evaluated. UV-Vis spectrophotometer showed absorbance peak in range of 420-435 nm. The ratio AgNO<sub>3</sub> and leaves extract 1:2.5 was optimal to synthesize AgNPs. The amount of AgNPs produced in solution was the highest when using PVA as a coating agent. The average size of AgNPs measured by DLS method was 40-60 nm, and by FESEM was 10-40 nm. Observing the solution of AgNPs after 3 months, we found that the solution was homogeneous, without precipitation. The synthesized AgNPs also showed the in vitro antibacterial activity against Pseudomonas aeruginosa. Thus, the Syzygium nervosum aqueous leaf extract can be used as a safe reducing agent for synthesis of AgNPs.

#### References

- [1] Z. Bedlovicova, A. Salayova, Bacterial pathogenesis and antibacterial control, 2017.
- [2] R. Kalaiarasi, G. Prasannaraj, P.A. Venkatachalam, 3 (2013), 8052.
- [3] A. Roy, O. Bulut, S. Some, et al., RSC Advances, 9 (2019), 2673.
- [4] M. Rai, A. Yadav and A. Gade, *Biotechnol. Adv.*, 27 (2009), 76.
- [5] G.N. Pham, T.T.T. Nguyen, H. Nguyen-Ngoc, Evidence-Based Com. And Alter. Medicine 2020 (2020) 14.
- [6] J.-C. Su, S. Wang, W. Cheng et al., The Journal of Organic Chemistry, 83 (2018), 8522.
- [7] P. T. M. Nguyen, N. Schultze, et al. Asian Pacific Journal of Tropical Biomedicine, 7 (2017) 43.

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# Ab-initio study of the magnetic properties of the double perovskites $A_2MM'O_6$ compounds, where A = alkaline earth or rare-earth metal and M, M' = transition metals

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The double perovskites (DPs)  $A_2MM'O_6$  (A = alkaline earth or rare-earth metal; M, M' = transition metals) oxides are considered as a material-class of interest due to both the chemical flexibility and the vastness of compositional and configurationally space spanning [1]. These materials exhibit also many valuable properties, for example, ferromagnetism above room temperature [1] being good candidate magnetocaloric materials [2], as well as high-performing semiconducticity for optoelectronic applications [3].

In this work, I would like to outline my aims and objectives of my PhD thesis, which is currently realized at the Doctoral school, Pedagogical University of Cracow and Institute of Low Temperature and Structure Research-PAN in Wrocław. Mostly, we focus on three groups of DPs compounds: i) magneto-caloric (Nd<sub>2</sub>NiMnO<sub>6</sub>, A<sub>2</sub>FeCrO<sub>6</sub> (A = Er, Tm)), ii) optoelectronic (A<sub>2</sub>LuTaO<sub>6</sub> (A = Ba, Sr), A<sub>2</sub>InSbO<sub>6</sub> (A = Ca, Sr, Ba), Ba<sub>2</sub>Zn<sub>1-x</sub>Ni<sub>x</sub>WO<sub>6</sub>), and iii) semiconducting (La<sub>x</sub>Sr<sub>2-x</sub>TiFeO<sub>6</sub>, A<sub>2</sub>MnWO<sub>6</sub> (A = Ba, Pb), La<sub>2</sub>FeMO<sub>6</sub> (M = Co, Rh, Ir)). For these compounds, we would like to determine electronic properties involving magnetic ground states (MGS), densities of states (DOS), electronic band structure (EBS), Fermi surfaces (FS), Electron Localization Function (ELF) of A<sub>2</sub>MM'O<sub>6</sub>, and optical properties. In order to accomplish the task we perform DFT calculations using the Full-Potential Linearized Augmented Plane Wave (FP-LAPW) method implemented in ELK code [4] and the Pseudo-Potentials Projector-Augmented Wave (PP-PAW) method implemented in Quantum-ESPRESSO simulation package [5].

Within the framework of the PhD thesis, by means of systematic studies, we hope to establish meaningful factors governing the observed physical properties in these compounds.

### References

- [1] D. Serrate, et al., *Double perovskites with ferromagnetism above room temperature*, J. Phys.: Condens. Matter 19 (2006) 023201.
- [2] A. Barman, et al., Caloric effects in perovskite oxides, Adv. Mater. Interfaces 6 (2019) 1900291.
- [3] E. Greul, et al., Highly stable phase pure Cs<sub>2</sub>AgBiBr<sub>6</sub> double perovskite thin films for optoelectronic applications, J. Mater. Chem. A 5 (2017) 19972-19981.
- [4] J. K. Dewhurst, et al., Elk code, version 7.2.42, URL http://elk.sourceforge.net/ (2021).
- [5] P. Giannozzi, et al., *QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials*, J. Phys.: Condens. Matter 21 (2009) 395502.

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## New study on the age of tertiary sediments in the Yen Bai basin (Northern Vietnam) based on palynological analysis

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The Red River Fault Zone (RRFZ) (Fig. 1A) is a reputed region of geotectonic interest. One of the most important topics in this area is the age of the sedimentary basin infills including Yen Bai Basin (YBB) (Fig. 1C), formed along the RRFZ, which is the key tectonic structure separating South China from the Indochina block (Fig. 1A) as well as NW Vietnam from NE Vietnam (Fig. 1B). The precise age of YBB has been under discussion for a long time. The previous concept assumed Miocene age of the infilling of this basin, however Oliwkiewicz-Miklasińska (2004) (after Nguyen et al. 2018) [1] found Oligocene and Miocene microflora in samples from single exposures in the basin.

Palynological analyses were carried out on thirty samples from five characteristic areas of the YBB. Almost all observed samples are lacking or very poor of spores and pollen grains. Only one sample is rich in pollen grains. The palynological assemblage of this sample is characterized by the strong dominance of angiosperm pollen. The angiosperm component is dominated by *Periporopollenites* and *Ulmipollenites*. Gymnosperm pollen mainly includes *Pinuspollenites*. Spores are very rare, including *Polypodiaceaesporites* and *Baculatisporites*. The assemblage has quite low taxonomical diversity. Most of the recognized taxa indicate a warm-temperate climate. The presence of *Pediastrum* algae indicates that the sediment was deposited in a shallow, standing fresh-water.

Basing on comparison with palynofloras from the vicinity, the composition of the assemblage corresponds well with the Eocene-Early Oligocene pollen assemblage of the Maoming Basin from Southern China. Common for both palynofloras are: dominance of angiosperm pollen with high frequencies of *Liquidambar* (*Periporopollenites*) and *Ulmus* (*Ulmipollenites*), poor of spores, mainly including *Pteris* (*Polypodiaceoisporites*), and medium frequency of gymnosperm pollen, mainly involving *Pinus* (*Pinuspollenites*). This palynological analysis may point to the evidence that the sediments of the Yen Bai Basin were deposited in the Eocene-Early Oligocene, which is in good relation with the results of Wysocka et al. 2018 [2], and 2020 [3]. This result would not only clarify the Con Voi Belt (Fig. 1B, C) exhumation but also provide a scientific basis for the the tectonic evolution of the RRFZ during Tertiary period.

On the other hand, the shortage of spores and pollen grains in collected samples is probably caused by weathering. Thus, the prospect of investigation in the YBB will implement to collect the better palynological samples.

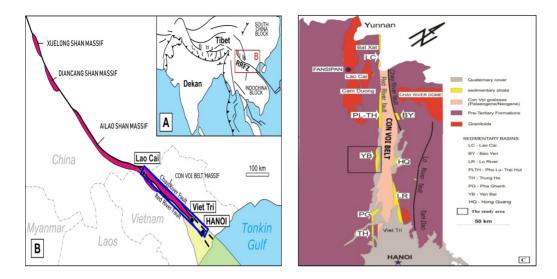


Figure 1. Location of the study area (after Nguyen et al. 2018)
(A) Position of the Red River Fault Zone in SE Asia;
(B) Location of massifs composed of high-grade metamorphic rocks;
(C) Position of the Yen Bai Basin along the Con Voi Belt

#### References

- [1] Nguyen Quoc Cuong, Phan Dong Pha and Hoang Van Tha (2018). An introduction to the Cenozoic tectonics of the Red River Fault Zone (Vietnamese part). GEOSEA XV Proceeding, Hanoi.
- [2] Wysocka A., Pha D.P., Durska E., Czarniecka U., Thang D.V., Filipek A., Cuong N.Q., Tuan D.M., Huyen N.X. and Tha H.V. (2018). New data on the continental deposits from the Cao Bang Basin (Cao Bang-Tien Yen Fault Zone, NE Vietnam)-biostratigraphy, provenance and facies pattern. Acta Geologica Polonica **68**(4), 689-709.
- [3] Wysocka A., Pha D.P., Durska E., Czarniecka U., Thang D.V., Filipek A., Cuong N.Q., Tuan D.M., Huyen N.X., Tha H.V. and Staniszewski R. (2020). The Na Duong Basin (North Vietnam): A key for understanding Paleogene basin evolution in relation to the left-lateral Cao Bang-Tien Yen Fault. Journal of Asian Earth Sciences **195**, 104350.

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## MeV ion-beam for analysis and modifications of materials: the crystallinity and stability of the Fe<sub>3</sub>O<sub>4</sub>-based thin films

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The MeV ion-beam has been used not only as the analytical tool (known as Ion beam analysis (IBA)) in e.g. microelectronics, nanotechnology, engineering and medicine, but also used for materials synthesis and modification of materials properties (known as Ion Beam Modification of Materials (IBMM)). The advantage of IBA is its high accuracy in determination of the chemical composition of materials, its non-invasiveness (in most cases), high speed of measurements, and in particular the possibility of a simple qualitative and quantitative interpretation of the obtained experimental results by using the computer simulations [1].

Magnetite (Fe<sub>3</sub>O<sub>4</sub>) is the earliest known magnetic material. It is one of the few exceptions among simple metal oxides, being a conductive material with interesting properties and has a wide application in technology for many years. It is referred as a half-metallic ferrimagnet having a full spin polarization at the Fermi level and has a high critical temperature (the Néel temperature  $T_{\rm N}=858{\rm K}$ ). Thus it is viewed as a promising candidate for spintronic application at room temperature.

Magnetite thin films have novel functionalities, which become a key ingredient for new concepts in catalysis and spintronic devices utilizing the spin polarized current [2]. Despite great efforts focused on the study of magnetite-based thin film systems, there is still a lack of information on the properties of the interfaces and the stability of Fe<sub>3</sub>O<sub>4</sub>-based systems under the influence of variable external conditions, such as the high temperatures, the exposure to high-energy ions, and/or the long-term exposure to air.

We aim at underlining the influence of thermal annealing and ion beam irradiation on the crystallinity and stability of epitaxial magnetite thin films prepared by molecular beam epitaxy (MBE) technique. The experiments have been carried out on different films with single and bilayer structure grown on MgO(001) single crystals, with the layer thickness in the range of 10-100 nm. The films in different states were investigated: after deposition (as-grown state), after exposure in air (ageing), after undergoing a thermal annealing and after a 1MeV Ar<sup>+</sup>, Kr<sup>+</sup> and Au<sup>+</sup> ion irradiations.

Our results revealed that the single-layer films (Fe<sub>3</sub>O<sub>4</sub>/MgO(001) has always a high crystallinity. For the bilayer films (Fe<sub>3</sub>O<sub>4</sub>/Fe/MgO(001)), on the film surface is always the stoichiometric Fe<sub>3</sub>O<sub>4</sub> layer, since the Mg out-diffusion (into the Fe<sub>3</sub>O<sub>4</sub> layer) is prevented by the Fe buffer layer. In some case, the large mismatch at the Fe<sub>3</sub>O<sub>4</sub>-Fe and Fe-MgO interface may influence the film crystalinity [3] (Fig.1).

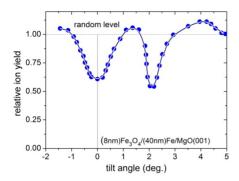


Fig. 1. The (normalized) channeling angular ion yield curve revealing two anomalies related to the channeling effect of Fe in the Fe<sub>3</sub>O<sub>4</sub> layer (wide minimum) and in Fe layer (narrow minimum) with respect to the [001] direction of the bi-layer (8 nm)Fe<sub>3</sub>O<sub>4</sub>/(50 nm)Fe/MgO(001) film. The angle difference between the minima indicates that the orientation difference of the Fe rows in those layers is two degrees.

The most important outcome of our work is finding the high stability of the  $Fe_3O_4$  layer on the bilayer-film surface upon 1 MeV Ar<sup>+</sup> i Kr<sup>+</sup> and Au<sup>+</sup> irradiations. For all investigated films, despite of a large decreasing of the layer thickness and even a full oxidization of the Fe buffer layer, the surface  $Fe_3O_4$  layer is always preserved upon ion irradiations with ion fluence of e.g.  $20.7 \cdot 10^{16}$  Ar<sup>+</sup>/cm<sup>2</sup>,  $5.0 \cdot 10^{16}$  Kr<sup>+</sup>/cm<sup>2</sup> (Fig. 2) and/or  $1.0 \cdot 10^{16}$  Au<sup>+</sup>/cm<sup>2</sup> [4].

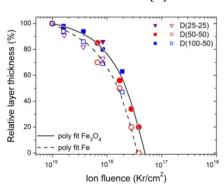


Fig. 2. Relative change (%) of the layer thickness for three bi-layer  $Fe_3O_4/Fe/MgO(001)$  films as a function of  $Kr^+$  fluence upon 1MeV  $Kr^+$  ion irradiation (D(25-25), D(50-50) and D(100-50); with the layer thickness in [nm] denoted by the number in the parenthese). The Fe buffer layer was fully oxided upon  $3.8x10^{16}$   $Kr/cm^2$ , whereas the stoichiometry of the surface  $Fe_3O_4$  layer is still preserved. The  $Fe_3O_4$  layer is expected to be destroyed upon irradiation at  $> 5.0\cdot10^{16}$   $Kr/cm^2$ .

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#### **References:**

- [1] Nastasi M., Mayer J.W., Wang Y. (2014). *Ion Beam Analysis: Fundamentals and Applications*. (CRC Press-Taylor and Francis Group). ISBN 9780367445843.
- [2] Parkinson G.S. (2016). Surf. Sci. Rep. **71**, 272-365.
- [3] Kim-Ngan N.-T.H. et al., (2017). Adv. in Nat. Sci.: Nanosci. Nanotech. 8(1), art. 045005.
- [4] Kim-Ngan N.-T.H., Krupska-Klimczak M.A. (2021), *Rozpraszanie wsteczne Rutherforda w cienkich warstwach magnetytu*. Wydawnictwo naukowe Uniwersytetu Pedagogicznego. 177 str. p-ISBN: 978-83-8084-647-0. e-ISBN: 978-8084-648-7

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# Assessment of the risk of Lead exposure when consuming *Siganus fuscescens* (Houttuyn, 1782) in the coastal of Quang Binh, Vietnam

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Siganus fuscescens (Houttuyn, 1782) usually live on the coast, they have delicious meat, rich in nutrients, and are high in Omega 3, so they should be consumed a lot [1]. In the aquatic environment, they often have a high position in the food chain, so they tend to accumulate large amounts of pollutants, such as lead [2]. Besides providing important nutrients for humans, it is also the risk of lead being taken into the human body through the consumption of the digestive tract. Lead is one of the toxic heavy metals, which is non-essential for the biochemical processes of any living animal [3].

From July to October 2019, a total of 50 individuals of *Siganus fuscescens* were collected at 5 different locations in the coastal of Quang Binh province. The liver, gills, and muscles were dissected and analyzed for lead content by flame atomic absorption spectroscopy, at the Institute of Biology, Pedagogical of Cracow University, Poland. The average concentration of Pb in most of the studied samples was less than the limit set by the Ministry of Health of Vietnam (MOH) and WHO (Table 1).

*Table 1. The concentration of lead in tissues of Siganus fuscescens (µg/g w.w)* 

Location	Tissue	Mean	Min	Max	SD
Canh Duong	Liver	0.220	0.087	0.412	0.113
	Muscle	0.083	0.013	0.207	0.065
	Gills	0.117	0.033	0.207	0.063
Quang Phuc	Liver	0.190	0.018	0.319	0.121
	Muscle	0.043	0.010	0.108	0.040
	Gills	0.101	0.019	0.207	0.074
Duc Trach	Liver	0.184	0.018	0.399	0.124
	Muscle	0.074	0.013	0.212	0.075
	Gills	0.050	0.018	0.108	0.037
Nhan Trach	Liver	0.177	0.027	0.304	0.089
	Muscle	0.048	0.007	0.206	0.071
	Gills	0.069	0.017	0.108	0.041
Nhat Le	Liver	0.321	0.213	0.428	0.080
	Muscle	0.114	0.009	0.212	0.068
	Gills	0.185	0.017	0.414	0.174

Pb content in the tissues of *Siganus fuscescens* decreased in the following order: liver > gill > muscle (p<0.05). The Estimated Daily Intake values were below the Provisional Tolerable Daily Intake thresholds set by the MOH and WHO. There was no risk to health when consuming Siganus fuscescens in coastal Quang Binh province at the time of the study.

#### References

- [1] R. Froese and D. Pauly, (2019). Mottled spinefoot Siganus fuscescens (Houttuyn, 1782). Retrieved May 31st, 2020 from https://www.fishbase.se/summary/Siganus-fuscescens.
- [2] D. Jiang, Z. Hu, F. Liu, R. Zhang, B. Duo, J. Fu, Y. Cui, & M. Li, (2014). Heavy metals levels in fish from aquaculture farms and risk assessment in Lhasa, Tibetan Autonomous Region of China. *Ecotoxicology* 23(4), 577-583.
- [3] P. J. Landrigan and A. C. Todd, (1994). Lead poisoning, Western Journal of Medicine 161(2) 153.

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# Effects of mulch C/N ratio and decomposition stage on plant N uptake and N availability in soil with or without wheat straw incorporation

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Mulches can improve soil properties, but little is known about nutrient availability in mulched soil that contains plant residues and the effect of mulching with manures. The aim of this study was to determine the influence of mulching with high or low C/N organic materials, in which low C/N materials differed in decomposability, and the presence of wheat straw in the soil on plant growth and N uptake, soil N availability and microbial biomass N within about four months after mulching. Three organic materials were used: mature wheat straw (W, C/N 80), young faba bean shoots (FB, C/N 7) and sheep manure (SM, C/N 8). There were eight treatments differing in amendment methods (mulching or mixing with W or both) and mulching materials (W, FB or SM). Treatments that were only mulched with W, FB or SM, are referred to as m-treatments. In m/s-treatments, after W was mixed into the soil, W, FB or SM were placed on the soil surface as mulch. Two other treatments included an unamended control and soil mixed with W. Wheat was planted 0, 35 or 70 days after mulching (referred to as 0, 35 and 70 DAM) and grown for 35 days. Faba bean mulch increased shoot dry weight, shoot N uptake and available N compared to wheat or sheep manure mulch, particularly in the m-treatments. Shoot dry weight was higher in m-treatments than corresponding m/s-treatments with the same mulch type. Shoot N uptake was higher in 70 DAM than in 0 DAM in all treatments and 0.3 to three-fold higher in mtreatments than the corresponding m/s-treatments. Microbial biomass N was higher in 0 DAM than in 35 and 70 DAM in most treatments and up to two-fold higher in m/streatments than the corresponding m-treatments. Available N in m/s-treatments was two to six-fold higher than m-treatments in 0 DAM, but differed little in older mulch ages of W and SM.

It can be concluded that compared to soil with only mulch, mixing of wheat straw into soil reduced plant growth and N uptake, particularly in the early stages of mulching (0 and 35 DAM). However, the presence of wheat in mulched soil may provide a longer lasting source of N for plants and reduce the risk of N leaching from rapidly decomposing low C/N mulch due to greater microbial biomass N uptake than only soil with mulch.

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## Sustainable promotion of cultural landscape values in the Son river basin, Quang Binh, Vietnam

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The Son River is the largest tributary on the right side of the Gianh River (which is the largest river in Quang Binh province). It flows from the Phong Nha-Ke Bang World Natural Heritage site at an elevation of 1,350 meters. The Son River basin is not only living to more than 50,000 people, with many different ethnic groups living together but also rich in natural resources, biodiversity, and cultural and historical diversity. Thanks to the efforts of local authorities and communities, the typical values of tangible and intangible heritages have been preserved, protected, used, and promoted quite effectively (Breaking Drum Festival of the Ma Coong, Singing "Tuong Boi" of Kinh people in Khuong Ha, Den Nghe Festival, New rice Festival, Xuan Son Ferry Port relic, Ho Chi Minh trail, 20 Quyet Thang street, Mu Gia pass...).

However, economic development, the process of urbanization, industrialization, modernization, and climate change have threatened the existence of the cultural landscape in the Son river basin. Therefore, it is necessary to have appropriate policies and plans based on a national legal basis, scientific basis and practical experience in conservation, use and sustainable promotion of cultural landscape values successfully applied in domestic and abroad.

Accordingly, it is necessary to focus on improving the quality and efficiency of cultural activities; harmoniously handle the conservation and promotion of the cultural heritage values of the ethnic groups with economic development and sustainable tourism activities in the localities. Attach importance to implementing programs to restore and preserve several traditional art forms; preserve and promote the cultural heritage of ethnic minorities; and cultural values in religion and belief.

#### References

- [1] M. Antrop (2006). Sustainable landscapes: Contradiction, fiction or utopia? *Landscape and Urban Planning*, 75 (3–4):187–97. doi:10.1016/j.landurbplan.2005.02.014
- [2] L. H. Shu-Chun, P. S. William, Y. Pao-Ning (2017). Making a Cultural Landscape: The Case of Dongshan River Basin, Taiwan. *Society & Natural Resources*, 30:12, 1507-1522, DOI: 10.1080/08941920.2017.1364450

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# Research on the reproductive characteristics of the blood cockle (*Anadara granosa*) in the coastal areas of Quang Binh province

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The blood cockle of the family Arcidae, the subfamily Anadarinae, is a source of valuable protein in tropical seas [1], and is a mollusk with high economic value [2]. The blood cockle has been collected in the coastal areas of Quang Binh from May 2020 to May 2021 to study its reproductive characteristics, using the methods is being applied in the study of reproductive characteristics of mollusks by Toral-Barza [3] and Baron [4]. The analysis of 832 blood cockle samples showed that their blood cockles go through 4 stages of development, these stages are different in terms of oocytes and male sex cells.

- Stage I: The blood cockle has not developed gonads yet, sex cells are just formed, the nucleus is unknown, male and female can not be distinguished.
- Stage II: Scallops are maturing, gonads begin to develop, and have begun to differentiate between males and females.
- Stage III: The gonads develop and take up most of the leg muscles. The sperm are milky white, the ovules are pale yellow, and the blood cockles are preparing to lay eggs.
- Stage IV: The cockle has finished laying, the gonads are wrinkled, and only a few sperm and oocytes remain in the gonads..

The blood cockle matured for the first time in the 24 mm height group. They spawn all year round, concentrating from April to July. The absolute fecundity of cockles ranges from 443,214 to 2,013,400 oocytes, depending on the size of the female cockle. Research on the reproductive biology of blood cockle has great significance in raising and producing artificial blood cockle breeds, contributing to the protection of blood cockle resources in Quang Binh province.

### References

- [1] M. J. Broom (1985). The Biology and Culture of Bivalve Molluses of the genus Anadara. *ICLARM Stdy and Reviews.* (12): 37p.
- [2] H. T. B. Dao (2005). Reproductive biology and trial production of blood cockle artificial seed. Doctoral thesis. Nha Trang University of Fisheries, Nha Trang.
- [3] L. Toral–Barza, E.D. Gomez (1985). Reproductive cycle of the cockle *Anadara granosa* in Calatagan, Batanges, Philippines. *Journal of Coasal Research*, 1(3): 241-245.
- [4] J. Baron (1992). Reproductive cycles of the Bivalve Molluses *Atactodea striata*, *Gafrarium tumidium* and *Anadara scapha* in New Caledonia. *Aust.J.Mar.Freshw.Res.* 43: 393-402.

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### Specific methods for studying the interaction between cell membrane & environment under stressful conditions

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Membranes are a part of the cell that plays a crucial role in many cellular processes. They function as a barrier against substances' penetration into the cell, especially those that can contaminate it, like toxins. There are numerous methods available to diagnose toxins (like rapid tests), but they mostly describe concentration and presence in cells. In this presentation, the application of *in vitro* culture and Langmuir technique is presented as specific and precise methods in the membrane investigation. Discussed techniques can indicate i) the degree of damage to the membrane during stressogenic effects of toxins, ii) changes of membrane structure, especially lipid organization, iii) determination of physicochemical parameters for interaction of lipids with the environment (e.g. toxins), iv) also may be helpful to optimize cells' protection against toxins.

In the perspective of public health, mycotoxins such as zearelenone, (produced by *Fusarium* species; fungi), are noted as very harmful substances for plant [1, 2] and animal (human) cells [3]. Experiments performed on *in vitro* culture obtained from plant cells and a description of this method are presented. Membrane lipids, isolated from native cells, were used to investigate the membrane - zearalenone interaction *via* the Langmuir technique. On the basis of the Langmuir isotherms, physicochemical parameters of membrane structure changes are calculated, such as: the area in monolayers occupied by single lipid molecules; the surface pressure at which the layer collapsed; the static compression modulus - representing mechanical resistance against layer compression, modified by the influence of zearalenone. This data allows for a better understanding the possibility of reorganization inside the membrane initiated by toxin presence and recognition of the first stages of the reaction mechanism between zearlenone and membranes. It can be helpful in discovering methods for cell protection.

### References

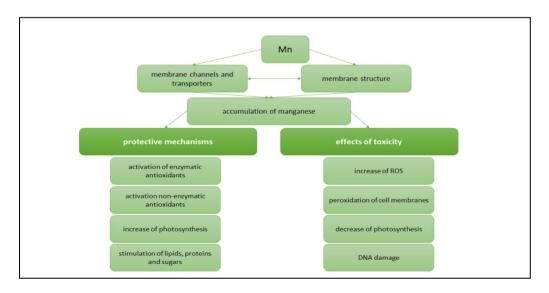
- [1] Filek, M., Sieprawska, A., Kościelniak, J., Oklestkova, J., Jurczyk, B., Telk, A., Biesaga-Kościelniak, J., Janeczko, A. The role of chloroplasts in the oxidative stress that is induced by zearalenone in wheat plants The functions of 24-epibrassinolide and selenium in the protective mechanisms. Plant Physiol Biochem. (2019),137:84-92.
- [2] Filek, M., Sieprawska, A., Oklestkova, J. Rudolphi-Skórska, E., Biesaga-Kościelniak, J., Miszalski, Z., Janeczko, A. 24-Epibrassinolide as a Modifier of Antioxidant Activities and Membrane Properties of Wheat Cells in Zearalenone Stress Conditions. J Plant Growth Regul (2018), 37, 1085–1098.
- [3] Barbasz, A., Rudolphi-Skórska, E., Filek, M., Janeczko, A. Exposure of human lymphoma cells (U-937) to the action of a single mycotoxin as well as in mixtures with the potential protectors 24-epibrassinolide and selenium ions. Mycotoxin Res. (2019), 35(1):89-98.

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### Evaluation of manganese as a stress factor in plant cells

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The development of industry is responsible for the release of significant amounts of metals to the environment i.a. during the processing of ores, production of non-rechargeable batteries or through the use of artificial fertilizers. Additionally, insufficient soils monitoring causes that plants uptake the micro and macroelements is determined by the dynamics of the environmental alterations. One of the essential metals necessary for the proper functioning of cells is manganese, which in elevated concentrations, may be toxic. As a result of the increased accumulation of this element, there is an overabundance of ROS generation, causing changes in the redox potential of cells, the modulation of the antioxidant enzymes activity, such as superoxide dismutases, peroxidases and catalases, consequently leading to the oxidation of molecules and their biological inactivation. The stressful effect of manganese ions depends on the concentration and time of exposure to this stress factor. Therefore, the aim of this presentation is to summarize the information about physiological and biochemical reactions in plants under Mn- stress.



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### Electrostatic interactions explain the higher binding affinity of the CR3022 Antibody for SARS-CoV-2 than the 4A8 Antibody

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A structural understanding of the mechanism by which antibodies bind SARS-CoV-2 at the atomic level is highly desirable as it can inform the development of more effective antibodies to treat Covid-19. Here, we use steered molecular dynamics (SMD) and coarse-grained simulations to estimate the binding affinity of the monoclonal antibodies CR3022 and 4A8 to the SARS-CoV-2 receptor binding domain (RBD) and SARS-CoV-2 N-terminal domain (NTD).

Consistent with experiment, our SMD and coarse-grain simulations both indicate that CR3022 has a higher affinity for SARS-CoV-2 RBD than 4A8's affinity for the NTD, and the coarse-grain simulations indicate the former binds three times stronger to its respective epitope. This finding shows that CR3022 is a candidate for Covid-19 therapy, and is likely a better choice than 4A8. An energetic decomposition of the interaction energies between these two complexes reveals that electrostatic interactions explain the difference in the observed binding affinity between the two complexes. This result could lead to a new approach of developing anti-covid-19 antibodies in which good candidates must contain charged amino acids in the area of contact with the virus.

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### Study of all-optical switching of 1560 nm femtosecond pulses using soft glass dual-core fibers

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All-optical switching has been intensively studied since the late 80s in order to enable signal processing and transmission rates at the level of Tb/s [1]. In 1988 Trillo et al. predicted that effective nonlinear solitonic switching can be performed in dualcore fibers (DCFs) [2]; however, all the subsequent experimental works were not successful due highly nonlinear transformations of the ultrashort pulses. Only recently, we have demonstrated experimentally a solitonic switching performance at 1560 nm wavelength using an all-solid DCF [3]. The fiber was made of two thermally-matched soft glasses synthesized in-house: the lead-silicate glass PBG-08 for the two cores, with a high linear (n = 1.945 at 1500 nm) and nonlinear ( $n_2 = 4.3 \cdot 10^{-19}$  m<sup>2</sup>/W) refractive indices, and the borosilicate UV-710 for the cladding, with lower refractive indices  $(n = 1.523 \text{ at } 1500 \text{ nm}, n_2 = 0.93 \cdot 10^{-19} \text{ m}^2/\text{W})$  [4]. We performed numerical analysis of the nonlinear propagation in such DCF with optimized structure, predicting high switching contrasts (> 15 dB) and sub-100 pJ switching energies. However, experimental results were not matching the numerical predictions both in terms of switching contrast and energy [5]. The reason of this discrepancy is the structural asymmetry of the fiber, which is inherently present after the stack-and-draw fabrication process [6]. This relates to the dual-core optical asymmetry. It means that the cores are distinguishable as slow and fast one with propagation constants  $\beta_s$  and  $\beta_{\rm f} < \beta_{\rm s}$ , respectively [3]. Under excitation of the fast (slow) core, a Kerr-induced phase shift decreases (increases) the mismatch  $\delta = \beta_s - \beta_f$  between the propagation constants of the cores. Therefore, the fast core excitation can support more efficient pulse redirection between the cores; nevertheless, this effect is accompanied by the coupling process, i.e. the nonlinear increase of the mismatch after the pulse redirection to the slow core.

We present two complex studies of all-optical switching of femtosecond pulses in the C-band (with central wavelength of 1560 nm). We used two different experimental techniques employed for two different DCFs: 1) self-switching, as presented in our previous paper [3], but using an all-solid DCF with lower DC asymmetry; 2) control/signal switching using the DCF presented in [7]. In the first case, the signal pathway is controlled nonlinearly by the intensity of the transported signal itself. In the second case, the redirection of a low-power signal is induced by another co-propagating pulse (control) with shorter wavelength. When using the less

asymmetric fiber, an effective self-switching of ultrafast low-energy pulses was demonstrated using 1560 nm, 75 fs solitonic pulses (Figure 1); in the case of more asymmetric fiber, a cross-switching of identical pulses was achieved driven by 270 fs, 1030 nm control pulses (Figure 2). The fiber length was optimized in both cases by the cut-back method. The self-switching approach employed in the case of less asymmetric fiber resulted in 35 mm optimal length, at which the highest switching contrast of 20.1 dB with broadband character in the spectral range 1450-1650 nm was observed. The cross-switching in the more asymmetric fiber was performed with even higher switching contrasts exceeding 25 dB at more homogeneous spectral dynamics in the C-band at 14 mm optimal length.

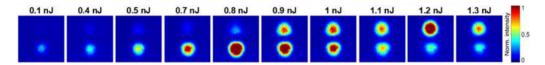


Figure 1. Infrared camera images of the output of the 35 mm DCF (bottom core excitation) under increasing input pulse energies, using the self-switching approach.

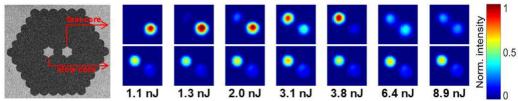


Figure 2. (a) (left) Cross-section of the DCF with higher asymmetry used for the dual-wavelength experiment. (right) Infrared camera images of the 1560 nm, 75 fs signal field at the DCF output under increasing energy of 1030 nm, 270 fs control pulses exciting the right (top series) and the left (bottom series) core with the combined beam.

Both outcomes represent high application potential with some complementary advantages. The simpler self-switching scheme requires only a single sequence of pulses and sub-nanojoule switching energy levels. However, in applications where even higher switching contrasts are required, the cross-switching can be performed by employing more complex experimental schemes with higher energy control pulses. To the best of our knowledge, the experimental results presented here disclose the highest switching contrasts in DCFs.

#### References

- [1] V. Sasikala, J. K. Chitra, J. Opt. 47(3) (2018) 307–317.
- [2] S. Trillo et al., Opt. Lett. 13(8) (1988) 672.
- [3] M. Longobucco et al., Opt. Fiber Technol. 63 (2021) 102514.
- [4] J. Cimek et al., Opt. Mater. Express 7(10) (2017) 3471.
- [5] M. Longobucco et al., Opt. Fiber Technol. 51 (2019) 48-58.
- [6] D. Pysz et al., Bull. Polish Acad. Sci. Tech. Sci. 62(4) (2014) 667–682.
- [7] M. Longobucco et al., J. Light. Technol. 39(15) (2021) 5111-5117.

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## Superconductivity and structure of selected 5*f* and (3-5)*d* metals and their hydrides

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Metallic uranium exists in three allotropic phases, between room temperature and its melting point:  $\alpha$ -U,  $\beta$ -U, and  $\gamma$ -U. The high-temperature  $\gamma$ -U phase with cubic structure can be retained to the room temperature by using a combination of ultrafast-cooling and alloying with 3d, 4d and 5d elements in groups IV - VIII of the periodic table

In this work, we summarize our investigations of the crystal structure and superconductivity of selected  $U_{1-x}T_x$  systems (U- n at.% T; x = n/100; at.=atomic percentage, T = Nb, Ru, Pt, Pd, Ti) prepared by ultrafast-cooling technique with the cooling rate of  $10^6$  K/s, i.e. U-T splats. The splat-cooling helps to reduce the necessary T concentration for retaining the cubic  $\gamma$ -U phase down to room temperature [1]. The investigated U-T alloys become superconducting with the critical temperature in the range of 0.40 - 1.95 K (Fig.1). Detailed investigations of the superconducting state at ultra-low temperature to 70 mK and in the magnetic field up to 5 T allows to determine the values of the upper critical field and the critical slope, which is respectively in the range of 1.0 - 4.3 T and 2.0 - 4.3 T/K [2.3].

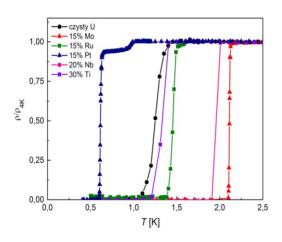


Fig. 1. Superconducting phase transition of selected U-T splats with  $\gamma$ -U phase revealed by abrupt drops of the electrical resistivity to zero. All curves are normalized to the resistivity value at temperature T=4~K.

The hydrogen absorption in  $U_{1-x}T_x$  splats (T = Nb, Ru, Ti) at high hydrogen pressures (exceeding 4 bar) leads to the formation of the hydrides  $(UH_3)_{1-x}T_x$ , consisted of  $\beta$ -UH<sub>3</sub> phase. They are ferromagnets with the Curie temperature in the range of 151 - 195 K, the spontaneous magnetization  $M_s$  in the range 0,80-1,05  $\mu_B/U$ .

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As common in all U hydrides, the hysteresis loops are very wide at low temperatures [4]. This feature is one of the striking effects resulting from very strong spin-orbit interaction in actinides, yielding high magnetocrystalline anisotropy (otherwise not so apparent in cubic systems) and consequently either strongly pinned narrow domain walls and/or monodomain grains with not easily reoriented magnetization. As usual, the coercivity fast decreases with increasing temperature. At the lowest temperature (T = 2 K) the remagnetization is reduced into a single step (Fig. 2). This can be understood as an avalanche effect of triggered by remagnetization of a single grain and propagating by exchange interaction over the grain boundaries.

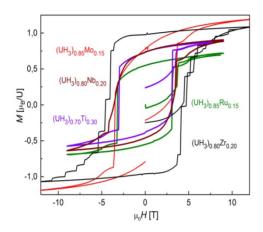


Fig. 2. Hysteresis loops of selected  $(UH_3)_{1-x}T_x$  hydrides. Most of them exhibit a single step at lowest temperature (2 K), except of  $(UH_3)_{0.80}Zr_{0.20}$  which reveals muliple steps.

### Acnowledgments

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#### **References:**

- [1] N.T.H. Kim-Ngan et al., J. Alloys & Comp. 580 (2013) 223.
- [2] S.Sowa et al., Physica B: Conden. Matter 536 (2018) 546-552.
- [3] N.-T.H. Kim-Ngan et al., Physica B 545 (2018) 152-158.
- [4] S. Sowa, PhD thesis (2021, in polish), Kraków.

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## A protein network for the prioritization of telomere interacting oncogenes associated with non-small cell lung cancer

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### Introduction

Recently, telomerase with its high specificity has emerged as an attractive target for anticancer drug development. Meanwhile, for such a complex disease like cancer, protein-protein interaction network (PPIN) is essential for understanding the whole landscape of disease pathway and resistance. In this study we revealed the telomere functioning crop of non small cell lung cancer PPIN with two subtypes (lung adenocarcinoma (LUAD) and lung squamous cell carcinoma (LUSC)) to identify the essential proteins in disease network.

#### Materials and methods

The TCGA [1] expression profile of telomere related genes first filtered by stages. Genes with differential gene expression between cancer and normal samples were further analyzed by a feature selection scheme modelling by iterated SVM – RFE. Through 100 loop feature selection, top ranking genes which have highest frequecies in optimal subsets were recruited to construct directed PPIN based on Inact database in iRefR package [2]. Finally, by minimum dominating set algorithm, we analyzed PPINs and classified the nodes as critical, intermittent, and redundant nodes.

### **Results and discussion**

In the first step, gene prioritization (Fig. 1A – F), generally, the size of optimal subsets is larger in LUAD than LUSC and increases with the increase of stage. Feature selection models exhibit the good performance. A few genes appear to be essential as they appear in all subsets with the absolute occurrence of 100. Especially, TGFBR2 is always in the best list for all stages of LUAD and two first stages of LUSC. Some genes such as CCT3 in LUAD and LPL in LUSC which are at top of three first stages. From small number of seed proteins, we built a relatively large PPINs especially stage IV of two subtypes (Fig. 1G – H). Critical nodes account for less than 40% of network size especially for two later stages of LUSC with the ratio of critical nodes of only about 10%. In total, 34 critical nodes as potential drug targets have been recognized across stages. Interestingly, proteins which are translated from genes in top ranking in feature selection are also critical in the networks. These proteins enriched on KEGG [3] (Kyoto Encyclopedia of Genes and Genomes) pathways with cut off p value of 0.05 and the results show that they involve in multiple pathways of cancers including non small cell lung cancer.

#### Conclusion

By iterated SVM – RFE and controllability analysis, we ranked the importance of telomere related genes on the discrimination of cancer and normal sample and explored the role of each protein in controllability of entire disease network. Also, we identified 34 telomere functioning crucial proteins as potential anticancer drug targets.

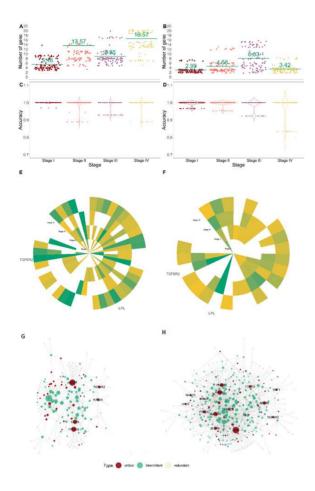


Figure 1. A - B: Size of optimal subsets in each iteration of feature selection (the blue horizontal line and its value represents the average of subset size) of LUAD and LUSC respectively. C - D: Classification performance feature selection of LUAD and respectively. E -LUSC Importance of genes in feature selection procedure of LUAD and LUSC respectively. G - H: Representative PPINs of two first stages of LUAD.

#### Acknowledgement

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### References

- [1] A. Colaprico, T.C. Silva, C. Olsen, L. Garofano, C. Cava, D. Garolini, T.S. Sabedot, M. Pagnotta, I. Castiglioni, M. Ceccarelli, G. Bontempi, H. Noushmehr, Nucleic Acids Res. 44 (2016) 1.
- [2] S. Razick, G. Magklaras, I.M. Donaldson, BMC Bioinform. 9 (2008) 405.
- [3] M. Kanehisa, M. Furumichi, Y. Sato, M. Ishiguro-Watanabe, M. Tanabe, Nucleic Acids Res. 49 (2021) D545.

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## Temperature dependence of anisotropic dielectric tensor of single-crystal α-SnS

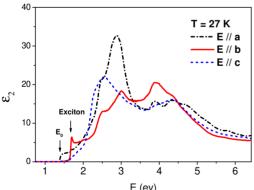
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Tin monosulfide (α-SnS) is well known as a natural p-type IV-VI binary compound for absorber material of the next-generation thin-film photovoltaic (PV) technology and thermoelectricity with abundant resources and better environmental compatibility. Because of the highly anisotropic structure, SnS shows a significant difference in optical and electrical properties in each direction. Knowledge of optical properties of materials plays an important role in the development of high-efficiency solar cells and thermogalvanic cells. In this work, we report the temperature dependence of the dielectric tensor of single-crystal α-SnS in spectral range from 0.74 to 6.42 eV and temperatures from 27 to 350 K by spectroscopic ellipsometry [1,2]. Figure 1 shows the imaginary parts of the dielectric tensor of single-crystal  $\alpha$ -SnS at 27 K. Especially, the appearance of excitonic feature in the armchair-direction (b-axis) at low temperature while it is disappeared in the others. Energy band structure of SnS with space group Pnma is shown in Fig. 2, which is calculated by using the mBJ method for band gap correction. By considering the electron-hole interaction, calculated results derived from the GW0 Bethe-Salpeter equation (BSE) are in good agreement with experimental data. We found that the excitonic feature is due to bandto-band transitions at a saddle point in the  $\Gamma$ -Y region, and is formed mainly from s and  $p_{\rm v}$  orbitals. The dominance of the fundamental band gap near 1.4 eV that occurs in zigzag-direction (a-axis) is due to band-to-band transitions in the  $\Gamma$ -X involving s and  $p_{\rm v}$  orbitals.



2 Exciton E<sub>0</sub>

Fig. 1: Imaginary parts of the dielectric tensor of single-crystal SnS along the principle axes at 27 K.

Fig. 2: Band structure of SnS calculated by the first principle with mBJ method for band gap correction.

#### References

- [1] V. L. Le et al., AIP Advances 10 (2020) 105003.
- [2] H. T. Nguyen et al., Sci. Rep. 10 (2020) 18396.

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### The mass problem in effective description of soliton motion

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A particular role for the modern description of nonlinear phenomena is played by structures such as solitons. In mathematical physics, the concept of soliton appeared in the work of N. Zabusky and M. Kruskal. At present, the concept of soliton is used to describe many phenomena appearing in the field of physics. In particular, in 1962 the British physicist B. Josephson presented a model describing the tunneling of Cooper pairs between two superconductors through a thin insulator layer. Currently, a system composed of two superconductors separated by a thin insulator layer is called a Josephson junction. In the description of the Josephson junction the equation (sine-Gordon) appears which also has soliton solutions including the so-called fluxon defined as soliton carrying the magnetic flux quantum.

The research concentrates on the dynamics of the fluxon in the Josephson junction. We consider the sine-Gordon model with translational invariance braking by the position dependent function F(x). The function F(x) represents the inhomogeneity, which is a kind of potential barrier for the fluxon propagating in the junction. The analysis of the interaction of the fluxons with the curved regions of the Josephson junctions in the framework of the collective variables approach is compared with exact results derived from the field equation. Three methods are considered. In the first one, the energy carried by the kink is analyzed and compared in homogeneous and inhomogeneous systems. The second approach is motivated by the perturbation scheme and the last one relies on the method of projection onto the zero mode of the system. In order to characterize the dynamical properties of the model, the critical velocity as a controlled physical parameter is considered. Investigations have revealed that in real system, only a part of the kink is involved in the interaction with an inhomogeneity. To verify this hypothesis, the mass correction depending on the curvature of the junction is proposed.

The Josephson junctions have found a wide variety of science and technical applications, and research into their possible further development is continuing. Fundamental for the preparation of junctions with specific properties are the descriptions of the soliton dynamics inside the junction. The results of the research could be the basis for future development of devices based on the Josephson junction and creation of electronics based on quantum effects occurring in the junction.

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### A review of ticks in Cracow, Poland's most popular tourist city

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Abiotic and biotic conditions in towns and cities create favourable circumstances for the propagation of many dangerous parasitic arthropods, i.e., vectors transmitting numerous diseases jeopardising both people and animals. Nowadays, ticks are one of the most dangerous vectors transmitting bacterial, viral and protozoan diseases. Walking through the areas of urban verdure as well as going sightseeing are vital for many humans' feeling of comfort. However, they are also zones wherein people may be exposed to ticks' attacks.

Cracow is one of Poland's most common destinations for tourists. The city's interesting and long history, numerous historic facilities, outstanding tourist attractions and lush green areas make it a very good choice for natives and foreigners from all around the world. Moreover, Cracow is the place with favourable conditions for the feeding of ticks, not only in the green areas rich in plants and on tourist tracks, but also inside buildings, on tops of buildings' towers and in the attics of antique rooms. From within 19 species of ticks with a constant existence in Polish fauna 5 have been recorded in Cracow: *Argas polonicus*, *Argas reflexus*, *Ixodes ricinus*, *Ixodes hexagonus* and *Dermacentor reticulatus*.

It is necessary to attract inhabitants' and tourists' attention, especially children's and adolescents', to ticks' habitats and to the rules of individual protection against their attacks. Furthermore, it is crucial to understand the risk of infection connected to the nature of green areas, access to a host and environmental conditions in towns and cities.

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# The risk of tick attacks *Ixodes ricinus* (Linnaeus, 1758) on selected tourist trails and educational-environmental paths in the Poprad landscape park

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In Polish fauna we encounter 19 species of ticks. The most common, with the biggest medical and veterinarian impact is *Ixodes ricinus*. It is necessary to examine the range of occurrence due to various diseases carried by ticks.

The Poprad Landscape Park is situated in the south of Poland in Małopolska (Lesser Poland). Because of its beauty and tourist facilities, The Park attracts tourists and local people all year round. In 2020 - 2021 the occurrence of ticks was checked in recreational areas, on tourists trails and educational-environmental paths of The Park. The first collection was conducted in May 2020 in Rytro, on the educational-environmental path "Rogasiowy Szlak" - 70 ticks were collected. Next collection was conducted in Rytro in June 2021 along the tourist trail "Barani Szlak" - 111 ticks were collected. The last collection was conducted in June 2021 in Krynica-Zdrój on the educational-environmental path "Na stoku Jaworzyny Krynickiej" - 32 ticks were collected. Each time, the collecting started at 8 a.m. or at 3 p.m within 4 or 5 examined areas. To collect ticks, the flagging method was used - low vegetation was swept with a flannel flag, which had been attached to the stick.

Collected ticks were placed in test-tubes filled with 70% ethanol. Then the taxonomic position and developmental stage of ticks were checked. The examinations conducted in recreational areas of The Poprad Landscape Park indicate the common occurrence of *Ixodes ricinus* and the possibility of spreading tick-borne diseases in the area of The Park. Therefore it is vital to educate and inform. Both locals and tourists should follow basic rules in order to protect themselves from ticks, especially during the spring and autumn peak of tick activity.

Ticks Ixodes ricinus



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### **Posters**

## The fixed point theorem in a banach space endowed with a digraph

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Following the extension of the Banach contraction principle in metric spaces endowed with a partial order for monotone or order preserving mappings initiated by Ran and Reurings [1], many mathematicians got interested into the investigation of the fixed point problem for monotone nonexpansive mappings. Results of this nature may be found in the articles [2, 3],... In 2018, Khamsi [4] affirmed that it is much more difficult to obtain similar results about the existence of fixed point of monotone nonexpansive if we replace a partially ordered set by a dighraph. Note that a partial order generates easily a digraph but not any digraph is generated by a partial order.

The purpose of this article is to extend the results of M. R. Alfuraidan and S. A. Shukri [5] concerning the fixed point theory for monotone nonexpansive mapping. In their work, they proved that if X is a uniformly convex Banach space endowed with a digraph G, then every G-nonexpansive mapping  $T: A \to A$  where A is a nonempty weakly compact convex subset of X, has a fixed point provided that there exists  $u_0 \in A$  such that  $T(u_0)$  and  $u_0$  are G-connected. By an argument analogous to R. Espínola and A. Wiśnicki used for their proof in the paper [6], we are going to show the existence of fixed points for monotone nonexpansive mapping in any Banach space endowed with a digraph. Alfuraidan and Khamsi used more a type function in uniformly convex Banach space to conclude the existence of a fixed point for G-nonexpansive mapping T. Our method is pure algebraic.

#### References

- [1] A.C.M. Ran, M.C.B. Reurings, *A fixed point theorem in partially ordered sets and some applications to matrix equations*, Proc. Am. Math. Soc. 132(5), 1435-1443 (2004)
- [2] M.R. Alfuraidan, M.A. Khamsi, *A fixed point theorem for monotone asymptotically nonexpansive mappings*, Proc. of the American Mathematical Society 146 (6), 2451-2456
- [3] M.R. Alfuraidan, M.A. Khamsi, *Fixed points of monotone nonexpansive mappings on a hyperbolic metric space with a graph*, Fixed Point Theory and Applications (2015) art. 44.
- [4] M.A. Khamsi, *Notes on Knaster-Tarski Theorem versus monotone nonexpansive mappings*, Moroccan J. of Pure and Appl. Anal., 4(1), 1-8 (2018)
- [5] M.R. Alfuraidan, S.A. Shukri: Browder and Göhde fixed point theorem for Gnonexpansive mappings, J. Nonlinear Sci. Appl. 9 (2016), 40784083
- [6] R. Espínola, A. Wiśnicki: *The Knaster-Tarski theorem versus monotone nonexpansive mappings*, Bulletin Polish Acad. Sci. Math. 66 (2018), 1-7.

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## First-principle study of electronic properties of IrSn<sub>4</sub> polymorphs

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Early investigations of the crystallography of the intermetallic IrSn<sub>4</sub> compound revealed the existence of three polymorphic modifications: i) trigonal form at low temperature, denoted as  $\alpha$ -IrSn<sub>4</sub> [1], ii) tetragonal form at high temperature marked as  $\beta$ -IrSn<sub>4</sub> [2,3] and iii) orthorhombic form at high pressure designated as HP-IrSn<sub>4</sub> [4,5]. Further, magnetic measurements of the  $\alpha$ -IrSn<sub>4</sub> [1] and  $\beta$ -IrSn<sub>4</sub> [3] pointed to the Pauli paramagnetic behaviour in both polymorphs. Surprisingly, a weak coupling superconductivity has been observed in the  $\beta$ -IrSn<sub>4</sub> phase only [3], since non-superconducting property was found in the  $\alpha$ -IrSn<sub>4</sub> variant [1].

In order to establish mechanism behind the superconductivity occurring in the  $\beta$ -IrSn<sub>4</sub> but not in  $\alpha$ -IrSn<sub>4</sub>, we undertook DFT calculations of the electronic structure properties involving densities of states (DOS), electronic band structures (EBS), Fermi surfaces (FS), Electron Localization Function (ELF). In this presentation, we compare the electronic properties between two polymorphs of IrSn<sub>4</sub>. The comparison implies that the reported superconductivity is governed by a strong correlation of the 5d-electrons.

### References

- [1] A. Lang and W. Jeitschko, J. Mater. Chem., 6, 1897-1903 (1996).
- [2] E-L. Nordmark, O. Wallner, U. Häussermann, J. Solid State Chem., 168 (1), 34-40 (2002).
- [3] V.H. Tran, Z. Bukowski, P. Wisniewski, L.M. Tran and A.J. Zaleski, J. Phys. Condens. Mater, 25 155701 (2013).
- [4] V. I. Larchev and S.V. Popova, J. Less-Common Met., 98 (1), L1-L3 (1984).
- [5] A.B. Künnen, D. Niepmann, W. Jeitschko, J. Alloys Compd., 309 (1-2), 1-9 (2000).

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# Synthesis and characterization of thermal conductivity of nanofluids based on Ag decoreated CNTs-graphene hybrid materials

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Currently, the development of nanotechnology has not only minimized the size but also improved the working speed of electronic devices. A large amount of heat generated during their working process at high power is a big problem which could be decrease their performance and lifetime. Therefore, reducing the working temperature is a key point to solve the problem.

There are several methods for heat dissipation, i.e. utilization of fans, thermal grease or fluids. Among the methods, fluid have been recieving great attention from scientist and manufactures due to its cost effective and fast heat exchange. Conventional fluids such ad water, ethylene glycol, oil, etc., are usually used as heat trasfer fluid. However, these basic fluids show low capability to transfer the heat due to their poor thermal conductivity. Several attempts have been made to improve their thermal conductivity. One of promissing method is adding solid nanoparticles into fluid, the heat transfer performance could be enhance, this new class of fluids called nanofluid. In this work, we present the nanofluid based on ethylene glycol containing silver nanoparticles decorated on the functionalized carbon nanotubes-graphene sheets hybrid materials (Ag/CNTs-Gr) was synthesized successfully by chemical reduction method.

The TEM, XRD, FTIR results show that Ag nanoparticles with an average diameter of 18nm were well decorated on the surface of both CNTs and graphene. The nanofluid containing 0.045 %wt of Ag/CNTs-Gr shows an enhancement in thermal conductivity of 76,4% at 60°C compare to the ethylene glycol. The enhancement due to the high thermal conductivity of CNTs, graphene and Ag nanoparticles as well as the higher surface area of Ag/CNTs-Gr hybrid structure.

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## Size-dependent geometric, electronic and H<sub>2</sub> adsorption properties of Ag<sub>n</sub>Cr (n=1-12) clusters

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An increasing interest has been paid for advanced alloy materials as promising candidates for solid-state hydrogen storage due to their low weight, low cost, and high storage capacity. Hydrogen (H<sub>2</sub>) interacting with metal clusters under well-controlled conditions can contribute to elucidate molecular level mechanisms for active sites of pure metal and alloy surface. In this respect, the geometric and electronic structures of bare and hydrogenated Ag<sub>n</sub>Cr clusters (n=1-12) have been studied using the density functional theory method. The results show that the Cr atom tends to occupy at the highest coordination position. The stability of studied clusters is not only governed by the symmetric geometry but also strongly depends on the electronic structure. In particular, the Ag<sub>12</sub>Cr dodecahedron is identified as a potential superatom in which the hybridization between 3d (Cr) and 4s (Ag) valence electrons forms a closed electron shell (1S<sup>2</sup>1P<sup>6</sup>1D<sup>10</sup>). The molecular orbitals were analyzed in combination with the electron shell model to clearly determine the nature of the interaction between the geometrical, electronic and magnetic structures. An analysis of the geometrical structure showed that the atomic coordination and steric factor of the Cr atom are the main influencing factors on the H<sub>2</sub> adsorption capacity of Ag<sub>n</sub>Cr. With a low energy barrier, the high reaction efficiency was achieved at sizes n=3, 4, and 5. The highest value was obtained at n=3 with an adsorption energy reaching 1.13 eV. The adsorption of H<sub>2</sub> molecules occurs mainly on the Cr atom. The interaction potential energy surface (PES), the kinetic states of the H<sub>2</sub> adsorption process are determined based on the vibrational frequency, energy, geometric structure and especially the results of intrinsic reaction coordinate (IRC) calculation.

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### Real-time, continuous-flow determination of the magnetic nanoparticles concentration by modified-GMR sensor

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Giant magnetoresistance (GMR) sensor shows excellent sensitivity and integration capabilities on devices, especially microfluidic systems. In this paper, a modified-GMR sensor has been integrated with microchannel and signal-processing circuit to determine magnetics nanoparticles (MNPs) concentration in the continuous flow by using Helmholtz coils magnetic field source. The GMR sensors was modified by using the laser technique and show the enhancement of the output signal and the system's sensitivity. The obtained results of 310 µm-reduced thickness GMR sensor system show that the sensivity was 826.67 mV/(mg.mL-1) and has increased by 1.32 times compared to the original sensor; and the limit of detection was also reduced respectively. This developed system appropriates to integrate into point-of-care microfluidic devices to detect biomolecule concentrations in real-time diagnostics. The approach allows fast identification and real-time analysis of the biomolecules conjugated with the magnetic nanoparticles (MNPs), which are essential requirements for various biomedical applications.

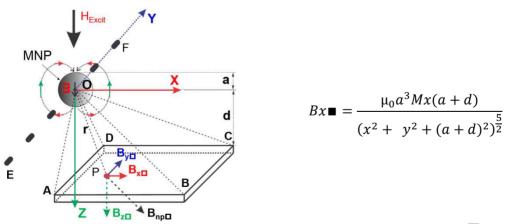


Fig 2. Schematic of the induced magnetic field generated by the MNP ( $Bx\square$ ) which depends on the distance from the center of the particle to the sensor's surface (z=a+d).  $Bx\square$  was also reported as inversely proportional to  $z^3$  in several recent articles. Many studies seek to reduce this distance to increase the sensitivity of the system.

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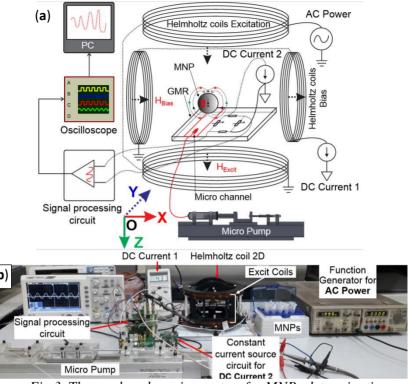


Fig 3. The employed sensing system for MNPs determination (a) Schematic diagram (b) Developed sensing system

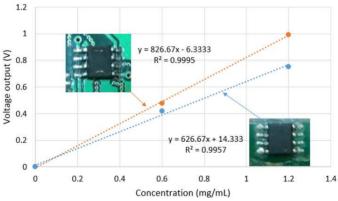


Fig 4. The response curve of modified and original GMR sensor with the various concentrations of MNPs

#### **References:**

- [1] K. Fodil et al, IEEE Trans. Magn. 49 (2013) 93-96.
- [2] K. Fodil et al, IEEE Trans. Magn. 50 (2014) 5300108.
- [3] K. Fodil et al, Appl. Phys. Lett. 108 (2016) 173701.
- [4] C.D. Damsgaard and M.F. Hansen, J. Appl. Phys 103 (2008) 6.

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## Sickest-first policy & predictive models for liver transplant candidates in the US

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The first successful liver transplant was performed on May 5, 1963. Thenceforth, liver transplantation for end-stage liver patients has gained worldwide acceptance as an established treatment saving thousands of lives annually. In the scope of our discussion, we will place our emphasis on the system of allocation livers for end-stage liver disease patients in the US. They used MELD-Na Score to determine how urgently patients need a transplant in order to rank them on a waiting list. Some patients may be able to receive donor's liver after a few weeks, but in some cases, the waiting time may be up to months or years.

In the second half of the discussion, we will talk about the use of Machine Learning techniques in improving the predictive model and the extendibility of the topic in assessing the fairness of the model toward demographic features such as gender or race, ...etc.

## References

- [1] Byrd, Jonathon & Balakrishnan, Sivaraman & Jiang, Xiaoqian & Lipton, Zachary. (2021). Predicting Mortality in Liver Transplant Candidates. 10.1007/978-3-030-53352-6\_31.
- [2] Bertsimas D, Kung J, Trichakis N, Wang Y, Hirose R, Vagefi PA. Development and validation of an optimized prediction of mortality for candidates awaiting liver transplantation. Am J Transplant. 2019 Apr;19(4):1109-1118. doi: 10.1111/ajt.15172. Epub 2018 Dec 6. PMID: 30411495.
- [3] {forester} R package: https://github.com/ModelOriented/forester
- [4] https://www.organdonor.gov/learn/organ-donation-statistics
- [5] Waiting List, MELD Score, Liver Transplants Dr. Robert S. Brown
- [6] Liver Transplant Waitlist, Part 1 | UCLA Transplantation Services
- [7] https://columbiasurgery.org/liver/liver-transplant-waiting-list
- [8] UNOS.org

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# Design a website for looking up diplomas and certificates on the website qbu.edu.vn

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Nowadays, the search for diplomas and certificates at Quang Binh University is being done manually. When students or employers want to verify the diplomas and certificates, they need to send a request letter to University for degree verification, the specialist who is in charge of diplomas and certificates must look up the register of original diplomas and certificates and then make an official dispatch to answer for students or employers. That process wastes time not only for students and employers but also for the University. Therefore, I came up with a solution to design a website that supports looking up diplomas and certificates.

The plan to implement this solution is:

- 1. Creating a database of diplomas and certificates
- 2. Building a website for diplomas and certificates which uses search algorithms to look up diplomas
- 3. Link the diploma lookup module on the homepage of the website qbu.edu.vn to the diplomas and certificates lookup website

Research results: The diplomas and certificates lookup website/ The website for looking up diplomas and certificates: http://qlvb.quangbinhuni.edu.vn/

Conclusion: this is an application which is suitable to the current practice of Quang Binh University. This application not only brings utility to users but also convenience for the university's work.

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# Change in electrical conductivity of river water due to the impact of small-scale hydroelectric system. Case study: Nida river, Poland

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The Electrical Conductivity (EC) of water is an indicator of water quality. EC is the ability to conduct an electric current in water, it reflects the amount of ions present in the water and depends on the physical properties and human activities in the river itself and in the watershed [1]. The construction of small-scale hydroelectric systems on rivers is quite common in Poland. On the one hand, these hydroelectric systems provide electricity for neighboring residential areas, partially solving electricity demand for local people. But on the other hand, they have many potential risks to the aquatic environment, affecting the surrounding ecosystem [2].

This study is based on determining then change in EC of water in the Nida River area, where a hydroelectric system is built, in order to assess the impacts of the hydroelectric system on the river water environment. The study has directly measured the EC and temperature of river water in the field, the river water area before and after the hydroelectric dam and a number of surrounding water channels flowing into the river. The results show that the EC of water has a relative difference between the measurement areas. The area behind the hydroelectric dam and the branches of the water channels have similarities. The area in front of the hydroelectric dam has an abnormally high increase in the EC of the water. This elevation can be explained by the long-term accumulation of water before the hydroelectric dam leading to the accumulation of minerals in the sediment and in the water. This accumulation may threaten the balance of river ecosystems and the lives of people in the surrounding area in the not too distant future.

## References

- [1] Patel, V., Parikh, P. (2013), Assessment of seasonal variation in water quality of River Mini, at Sindhrot, Vadodara, International Journal of Environmental Sciences, 3(5), 1425-1436.
- [2] Kucukali S (2014a) Environmental risk assessment of small hydropower (SHP) plants: a case study for Tefen SHP plant on Filyos River. Energy Sustain Dev 19:102–110

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# Combined ligand-based and structure-based virtual screening approach and molecular dynamics simulation of SARS-CoV-2 protease (Mpro and PLpro) for identifying antiviral inhibitors against SARS-CoV-2

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## Introduction

Severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) is the cause of the fatal global pandemic, COVID-19, leading to the discovery of potential compounds is urgently needed. In this scenario, the study focused on virtual screening of promising anti SARS-CoV-2 agents inhibiting 2 important antivial targets: main protease (Mpro) and papain-like protease (PLpro), those are essential for viral replication.

## Materials and methods

We proposed a screening method with multiple filers, base on experimental data of IC50 and computional method, simultaneously (Fig.1). 100 non-covalent inhibitors of Mpro and 91 non-covalent inhibitors of PLpro were collected with experimental IC50 data from previous published articles. Their molecular descriptors were calculated with AlvaDesc software version 2.0.2 [1] and then QSARINS software version 2.2.4 [2] was used to build 2D QSAR models. From Zinc database with 7.3 million compounds, QSAR models were applied to get top 100 ligands with highest predicted pIC50 of each model. These compounds and experimental molecules continued to be docked to 2 proteases (Mpro PDB ID: 7LMD; PLpro PDB ID: 7LBR) by

MOE 2009.10 software [3] and validated with MD simulation using the NAMD 2.13 package [4]. The best candidates are evaluated with Lipinski's rule of five and ADMET analysis to determine drug-like and pharmacokinetic properties.

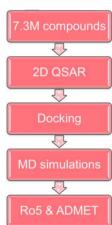


Figure 1: Flowchart of potential compounds parallel screening for Mpro and PLpro.

## **Results and discussion**

Both 2D QSAR models of Mpro and PLpro show appreciably high R2 value of training set (Mpro, R2 = 0.8944; PLpro, R2 = 0.9165). For internal validation, Q2 leave-one-out (LOO) was calculated (Mpro, Q2LOO = 0.8711; PLpro, Q2LOO = 0.8965). R2 of test sets were used for external validation (Mpro, R2ext = 0.8569; PLpro, R2ext = 0.8190). All parameters are good enough to show that these models could be used for screening (Fig.2).

The docking process was devided into 2 parts. First, the molecules from published articles which had experimental IC50 values of one protease were docked to another, to find out the compounds which could inhibit more than one target. **PL64** and **M88** show good experimental pIC50 and also best scores in the list (**PL64**, Exp.pIC50 = 5.96, score (Mpro-target) = -5.34; **M88**, Exp.pIC50 = 7.44, score (PLpro-target) = -9.75) (Fig.3 A,D). Second, the compounds from 2D QSAR screening were docked to their own protease. **1772818546** (score (Mpro-target) = -6.65, Pred.pIC50 = 7.97);

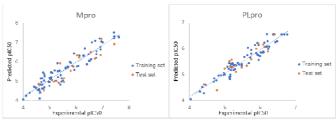


Figure 2: Plot of the predicted training set and test set vs experimental pIC50 values.

**301054495** (score (PLpro-target) = -7.76, Pred.pIC50 = 7.25) show potential for inhibition (Fig.3 B,E). Besides, **1687828** seemed to be a good candidate for dual-target inhibition (Mpro-target: score = -4.39, predicted pIC50 = 6.46; PLpro-target: score = -4.51, predicted pIC50 = 6.25) (Fig.3 C,F). Then we validated their comformations with MD simulation. The RMSD ranged from 1 to 3 Å indicated that all of them are stable in the complexes. For further Lipinski's rule of five and ADMET analysis, all 5 compounds are drug-like molecules and have favorable pharmacokinetic properties.

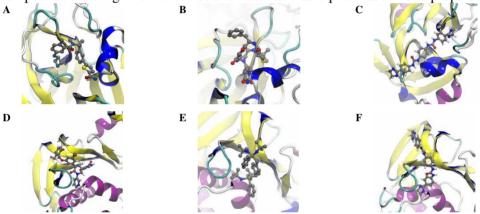


Figure 3: A-C: Docking poses of Mpro inhibitors at the active site (PL64, 1772818546, 1687828 respectively); D-E: : Docking poses of PLpro inhibitors at the active site (M88, 301054495, 1687828 respectively).

## Conclusion

From experimental data and zinc database with 7.3 million compounds, we had selected the best candidates for viral protease inhibition. All five compounds have potential for future drug development.

## References

- [1] Mauri, A. (2020). alvaDesc: A tool to calculate and analyze molecular descriptors and fingerprints. In K. Roy (Ed.), Ecotoxicological QSARs (pp. 801–820). Humana Press Inc. https://doi.org/10.1007/978-1-0716-0150-1 32.
- [2] Gramatica, P., Chirico, N., Papa, E., Cassani, S., Kovarich, S., QSARINS: A New Software for the Development, Analysis, and Validation of QSAR MLR Models. Journal of Computational Chemistry (Software news and updates) 2013, 34, 2121-2132, DOI: 10.1002/jcc.23361.
- [3] Molecular Operating Environment, MOE 2009.10; Chemical Computing Group Inc.: 1010 Sherbooke St. West, Suite #910, Montreal, QC, Canada, H3A 2R7, 2009.
- [4] J. C. Phillips et al., Journal of computational chemistry, 2005, 26, 1781–1802 E-mail of the presenting author: huylelhp@gmail.com

# A simple rule-based approach for designing novel dual-target AChE and BACE1 inhibitors as anti-Alzheimer agents

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## **Background**

Alzheimer's disease (AD) is a complex neuro disoder with many unusual risk factors and pathological mechanisms such as cholinergic hypothesis, amyloid- $\beta$  (A $\beta$ ) aggregation, and oxidative stress [1, 2]. Compounds acting on multi-targets could be of significant therapeutic benefit for AD.

### Method

In this direction, a rule-based machine learning approach based on classification trees was applied for the rational design of novel dual-target acetylcholinesterase (AChE) and  $\beta$ -site amyloid-protein precursor cleaving enzyme 1 (BACE1) inhibitors. To do so, a large data of 3524 compounds having AChE and BACE1 measurements was curated from the ChEMBL database [3]. A series of stand-alone and ensemble classification tree models based on CRT, CHAID and RF algorithms were developed to predict both AChE and BACE1 inhibitory activities using a pool of >3000 0-2D molecular descriptors implemented into Dragon software version 6.0.

## **Results**

As the results, 2 models and 2 multiclassification systems predicting AChE activity were obtained and displayed acceptable performance with global accuracy ( $Q^2$ ) ranged from 0.79-0.85 for training and 0.75-0.81 for test sets. Likewise, those obtained for BACE1 activity showed good performance with accuracy ranged from 0.79-0.83 for training and 0.77-0.81 for test sets. *F*-scores obtained for the training and test sets ranged from 0.78-0.85 for all the models, suggesting a balance level of precision and accuracy for discriminating active from inactive compounds.

Based on the best rules revealed from each tree, a set of 67 AChE and 144 BACE1 representative inhibitors were extracted and clustered according to the most important structural features. By selecting the most bioactive compounds from representative clusters, we identify 6 fragments for AChE and 6 for BACE1 inhibitors with the highest frequency that have positively influence on the biological activity. Based on these fragments, a new library of 120 inhibitors was designed and screened for dual-target AChE/BACE1 inhibitory activity.

Finally, eight compounds bearing piro-tetracyclic rings, furo[3,2-b]quinolines, furo[2,3-b:4,5-b']diquinolines and fatty amide chain were predicted to be potential inhibitors against dual-target. They were further examined for drug-like properties, especially those related to the blood-brain barrier passage.

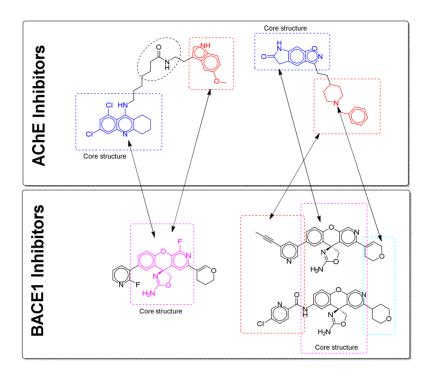


Fig. 1. Key fragments for designing novel dual-target AChE/BACE1 inhibitors

## References

- [1] Ibrahim, M. M. and Gabr M. T. (2019) "Multitarget therapeutic strategies for Alzheimer's disease", Neural Regeneration Research, 14(3), pp. 437–440.
- [2] Wang, Y., Wang, H., et al. (2016), "AChE inhibition-based multi-target-directed ligands, a novel pharmacological approach for the symptomatic and disease modifying therapy of Alzheimer's disease", Current neuropharmacology, 14(4), pp. 364-375.
- [3] Gaulton, A., Bellis, L. J., et al. (2012), "ChEMBL: a large-scale bioactivity database for drug discovery", Nucleic Acids Res, 40(Database issue): D1100–D1107.

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# Indication of soil water table of forest biogeocenosis of the Leningrad region using scales L. G. Ramensky

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### Introduction

The current state of the forest fund of the Leningrad Region is characterized by a significant share of secondary forests, as well as forests affected by various types of economic impact. For areas with a significant proportion of transformed forests and habitats, when distinguishing typological units, relatively stable features of soils and vegetation that characterize the ecological regimes of forest areas should be used more widely. Among the signs of vegetation, it is recommended to use, first of all, estimates on ecological scales, and for practical recognition of forest types in the field, ecological groups of plant species are recommended [1].

Dynamic processes in vegetation depend primarily on moisture conditions associated with the level of soil water table (SWT) and the intensity of infiltration of the water flow to the hydrogeological system. The shallow water table facilitates interaction with plant roots, supplies water to plants and, through fluctuations in the water table, affects the availability of oxygen and nutrients in the soil. At the same time, excessively prolonged flooding of root systems also adversely affects the state of woody plants, which is due to the inaccessibility of oxygen for the root systems, displaced from the soil pores by SWT. In turn, the vegetation affects the water balance of the soil through the dynamics of growth, transpiration and the interception of precipitation by the crowns. This strong relationship between vegetation and groundwater levels leads to an important and interesting feedback loop between hydrological and ecosystem processes. Understanding the relationship between SWT and vegetation is especially important in areas where forest development projects are implemented in wetlands and in artificially drained peatlands. In this regard, the value of express indication of the SWT regime for vegetation will increase.

## Material and methodology

The monitoring of the SWT level was carried out in wells on test plots (PP) laid in different types of forest growing conditions, types of forest and in clearings in Ontsevsky, Druzhnoselsky and Divensky uchastkovoye lesnichestvos of Siversky experimental demonstration forestry SPbNIILH (now Gatchinskoe lesnichestvo) in May, September 1 time in 5 days; in June, July, August every 10 days. The observations covered the following types of forest and types of clearings (the names are given according to [1]): oak grass spruce forest, spruce and oxalis aspen forest on loam and two-member sediments, spruce forest, birch forest, clearing on two-member sediments, 2 spruce forests and long-moss-blueberry felling on insufficiently drained sands and binomial deposits, 2 pine forests of ledum-blueberry pine forests on insufficiently and weakly drained sands, 2 sphagnum-blueberry pine forests on weakly drained loams and binomial sediments, sphagnum pine forest, sphagnum-cotton grass

pine forest on high peat moss silt-meadows flowing moistening, meadow-grass and bog-grass birch forests on loams with flow-through moistening, bog-grass pine forests on drained peat, 2 dried oxalis peat pine forests.

The observations were carried out by V.N. Fedorchuk and V.Yu. Neshataev in 1979-1985. A taxation description of the stand, undergrowth, undergrowth was carried out at the PP, the projective cover of species and layers of living ground cover was determined. According to the composition of the phytocenosis, taking into account the projective cover of the species, the degree of moisture was determined according to the scales of L. G. Ramensky [1]. For each PP, the average SWT level was determined in May and by decades, the average number of decades, during which the SWT level was observed above 20 cm from the surface.

## Results and discussion

Observations have shown that forest types are closely related to the level of SWT. Prolonged flooding of root systems during the growing season (10-15 decades) and a high level of SWT in May were observed in the sphagnum-cotton grass pine forest and marsh grass birch forest (about 2 cm above the soil surface), as well as in the meadowsweet birch forest (about 2 cm below the surface) ... It was found that in the clearings of blueberry long-moss-blueberry types of forest growing conditions, the number of decades, during which the SWT level was observed above 20 cm from the surface, is more by 2-3 decades than in forests.

Flooding of the 20-cm layer was not noted in the sorrel spruce forest and in the dried oxalis pine forest. The average ten-day SWT level in May in these forest types was 76 and 44 cm, respectively. A deep level of SWT in May is also typical for the oak-grass spruce forest 77 cm, but in the autumn period in this type of forest flooding of the 20-cm layer was observed for 5 days.

The closest connection by the method of correlation analysis was established between the level of moisture (Y), determined according to L. G. Ramensky's scales, and the number of decades during which the level of SWT was observed above 20 cm from the surface (Figure 1). The high coefficient of determination makes it possible to assert that the stages of moistening, determined by the composition of the phytocenosis according to the scales of L. G. Ramensky's, are closely related to the regime of SWT.

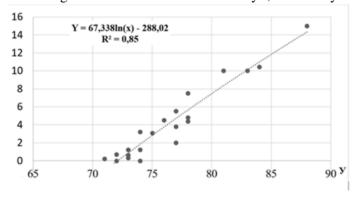


Figure 1. The relationship between the level of SWT and humidification according to the L.G. Ramensky (negative values - for SWT, standing above the soil surface).

### Reference

[1] Fedorchuk V.N., Neshataev V.Yu., Kuznetsova M.L. Forest ecosystems of the northwestern regions of Russia: Typology, dynamics, economic features. SPb. (2005) 382. E-mail of the presenting author: khanhvudhsp@gmail.com

## Production of sodium hypochlorite by direct electrolysis of seawater with OIPTA + TA electrode

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In this study, the preparation of sodium hypochlorite by the OIRTA + TA electrode was carried out in a cylindrical electrochemical cell. Studies have determined the effect of the optimal current density of diaphragmless electrolysis of the water of the Vietnamese Sea to obtain sodium hypochlorite. A non-diaphragm flow-through electrolysis cell is used to study the effect of flow rate and current density on the concentration of active chlorine in the resulting hypochlorite, voltage, pH, electrolyte temperature and the change in the current efficiency of chlorine and power consumption/kg of active chlorine formed. The minimum specific energy consumption of 3-4 kWh/1 kg of the generated one can be obtained when the concentration of active chlorine in the generated hypochlorite is in the range from 1.0 to 2.0 g/dm³. At the same time, the current output of chlorine also reaches its maximum values and is 68-95%, which determines the technological and economic feasibility of obtaining sodium hypochlorite from seawater.

#### References

- [1] E. M. Elsayed, A. E. Saba. Int. J. Electrochem. Sci. 4 (2009) 627.
- [2] M. Saleem. J. Chem. Soc. Pak. 33 (2011) 295.
- [3] A.M. Polcaro, A. Vacca, M. Mascia, S. Palmas, R. Pompei, S. Laconi. Electrochimica Acta, 2007 52 (7) 2595-2602
- [4] C. Liang, N. Huang J. Mater. Eng. Perform., 18 (2009) 1086-1090
- [5] Л. Н. Фесенко, С. И. Игнатенко, Водоснабжение и канализация. (2009) 97-103.
- [6] Фесенко Л.Н., Игнатенко С.И., Пчельников И.В., Косолапова С.В., Геркен А.Е., Технологии очистки воды «ТЕХНОВОД-2016»: материалы IX Межд.. научн.-практ. конф., г. Ростов-на-Дону, (2016) 157-165.

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## Factors affecting ecotourism development of Hac Hai lagoon, Quang Binh province

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Ecotourism is a type of tourism that creates an organic and harmonious relationship between people and nature, promoting the sense of responsibility of people for environmental protection. Developing ecotourism has become the current trend of sustainable tourism development in our country in particular and the world in general.

Hac Hai Lagoon, locates in the downstream of Kien Giang river - along 2 districts of Quang Ninh and Le Thuy, Quang Binh province. It is known as a lagoon with a variety of rich and diverse seafood such as shrimp, crab, etc and the sparkling, immense, poetic natural scenery with many natural conditions to develop eco-tourism.

Based on the study of 6 factors: (i) economic resources, (ii) natural resources, (iii) socio-cultural resources, (iv) environmental resources, (v) management policy tourism management, (vi) human resources, the author proposes some solutions to develop eco-tourism in Hac Hai lagoon.

### References

- [1] Buckley, R. (1994). A framework for ecotourism. *Annals of tourism research*, 21(3), 661-665.
- [2] Ha, T. H. (2013), Research and development of community-based eco-tourism in fishing villages on Ha Long Bay, University of social sciences and humanities.
- [3] Ho, T. T. K (2017), Proposing a model of environmental protection associated with ecotourism and sustainable livelihoods for the salt craft village of Ly Nhon commune, Can Gio district.
- [4] Nguyen, V. H. (2002), Research and assessment of ecology and environment in the lower Kien Giang river for sustainable development.
- [5] Nguyen, T. A. H. (2007), Research on environmental factors for aquaculture development planning in Hac Hai lagoon, Quang Binh province.
- [6] Tao, T. C. H. (2006). Tourism as a livelihood strategy in indigenous communities: Case studies from Taiwan.
- [7] Tran, D. H. (2007), Research on operating process of My Trung sluice gate to ensure prevention of salinity, waterlogging, environmental protection, sustainable development
- [8] Shen, F., Hughey, K. F., & Simmons, D. G. (2008). Connecting the sustainable livelihoods approach and tourism: A review of the literature. *Journal of Hospitality and Tourism Management*, 15(1), 19-31.

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# Highly enhanced adsorption for the removal of Ag (I) from aqueous solution by Mercaptoethylamine functionalized vermiculites

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Silver has good malleability, ductility, photosensitivity, electrical and thermal conductivity, it is widely used in electroplating, batteries, film, and other fields; long-term exposure to silver compounds may cause liver and kidney damage. Currently, commonly used methods of processing silver include the ion exchange method, electrolysis method, and membrane separation method. However, these methods generally have the disadvantages of high processing cost and high operating cost. Due to its simple operation, high adsorption efficiency, and various types of adsorbents, the adsorption method has been widely used in the treatment of various wastewater with excessive heavy metal content [1-4]. As a universal adsorption material, clay minerals have abundant reserves and low prices, high specific surface area, and environmental friendliness [5].

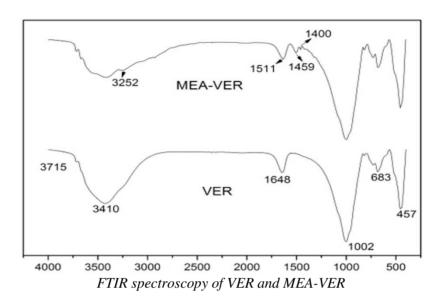
Vermiculite is often used as an adsorbent for the management of environmental pollution because of its advantages of abundant reserves, low prices, and environment friendly. However, the adsorption ability of heavy metals and organic matter in natural clay is poor. For the sake of the adsorption performance of natural clay, a lot of literature has studied different modification methods to improve the properties of clay such as pore size, specific surface area, thermostability, and chemical activity. In this study, raw vermiculite has been modified by 2-aminoethanethiol (MEA) to obtain organic vermiculite as an adsorbent for the removal of silver ions in an aqueous solution.

The physicochemical properties of the raw and modified vermiculites were analyzed by Fourier transform infrared (FTIR) spectroscopy, thermogravimetry-differential scanning calorimetry (TG-DSC) and BET analysis, which indicated that MEA was successfully grafted onto the vermiculite. Additionally, batch adsorption experiments involving initial pH, adsorbent dosage, time, and temperature demonstrated that the adsorption capacity of Ag<sup>+</sup> onto MEA-VER was improved highly compared with that of raw vermiculite. The optimum adsorbent dosage was 2.0 g/L, the adsorbents presented a high removal efficiency of Ag<sup>+</sup> in a wide range of initial pH values (1-5).

The kinetics studies showed that the adsorption process was described well with a pseudo-second-order model and the equilibrium was achieved at about 200min of contact time. The adsorption isotherm of Ag<sup>+</sup> onto vermiculites fitted the Langmuir model well. All these results indicated that the adsorption process onto vermiculites was taken place mainly by coordination and electrostatic adsorption.

Compared with the infrared spectrum of VER, MEA-VER has several new absorption peaks, where the absorption peaks at 1459, 1511, and 3252 cm<sup>-1</sup> represent the strain vibrations of -CH<sub>2</sub> or the bending vibrations of -NH<sub>2</sub> [6]; The absorption peak at 1400 cm<sup>-1</sup> represents the bending vibration of -CH<sub>2</sub> [7]. These absorption peaks

are characteristic absorption peaks of mercaptoethylamine, which indicates that mercaptoethylamine was successfully loaded into vermiculite.



#### References

- [1] Huisman, Jacco L., Gerard Schouten, and Carl Schultz. "Biologically produced sulphide for purification of process streams, effluent treatment and recovery of metals in the metal and mining industry." *Hydrometallurgy* 83.1-4 (2006): 106-113
- [2] Kim, Dong Seog. "The removal by crab shell of mixed heavy metal ions in aqueous solution." *Bioresource Technology* 87.3 (2003): 355-357
- [3] Fu, Fenglian, and Qi Wang. "Removal of heavy metal ions from wastewaters: a review." *Journal of environmental management*92.3 (2011): 407-418.
- [4] Montiel, Helena, et al. "Mathematical modelling of accidental gas releases." *Journal of Hazardous Materials* 59.2-3 (1998): 211-233.
- [5] Gonzalez-Munoz, Maria Jesus, et al. "Recovery of heavy metals from metal industry waste waters by chemical precipitation and nanofiltration." *Desalination* 200.1-3 (2006): 742-744.
- [6] Wu, Pingxiao, et al. "Characterization of organo-montmorillonites and comparison for Sr (II) removal: equilibrium and kinetic studies." *Chemical Engineering Journal* 191 (2012): 288-296.
- [7] Li, Zhaohui, Wei-Teh Jiang, and Hanlie Hong. "An FTIR investigation of hexadecyltrimethylammonium intercalation into rectorite." *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy* 71.4 (2008): 1525-1534.

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# **Evaluation of the immunostimulating effect of Milnavir capsules on experimental animals**

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Immune-stimulating drugs derived from herbs have recently been interested in research to support patients in the prevention of diseases such as cancer, viral diseases, respiratory diseases. This study was conducted with the aim of evaluating the immunostimulatory effects of Milnavir capsules in experimental animals.

Capsule preparation contains 500 mg of dried extracts of medicinal plants with equivalent composition including Astragalus membranaceus (Fisch) Bunge 1000 mg; Atractylodes macrocephala Koidz 500 mg; Ledebouriella seseloides (Hoffm.) H. Wolff 500 mg; Zingiber officinale Rosc 500 mg; Ligusticum wallichii Franch 500 mg; Gentiana macrophylla Pall. 500 mg; Cinnamomum cassia Presl 400 mg; Stemona tuberosa Lour 300 mg; Angelica dahurica (Fisch. ex Hoffm.) Maxim 300 mg; Notopterygium incisum K.C. Ting et H.T. Chang 250 mg; Glycyrrhiza uralensis Fisch. ex DC 250 mg.

Experimental animals are Swiss white mice, healthy, weighing 18 - 20 g. The recommended adult dose is 4 tablets/day, equivalent to 40 mg/kg/day. The dose conversion in mice (conversion factor is of 12) was 480 mg/kg/day. The evaluated indicators are the change in body weight, weight of spleen and thymus, white blood cell count and formula, some hematological indicators, serum cytokine levels of the experimental animals.

The results showed that Milnavir capsules at doses of 480 mg/kg/day and 960 mg/kg/day had immunostimulating effects, increasing mice body weight, spleen & thymus weight, white blood cell count, serum IL-2 and TNF- $\alpha$  levels in cyclophosphamide-induced white mice. This effect of Milnavir is equivalent to  $\beta$ -glucan 250 mg/kg/day.

Research results are promising for the use of Milnavir capsules in the prevention and treatment of influenza, viral respiratory infections.

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# Evaluation of regulating effect on exogenous dyslipidemia of capsules prepared from fermented Allium sativum, Hibiscus sabdariffa, Gynostemma pentaphyllum and Alisma plantago aquatica on white rats

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Dyslipidemia is a common disease in modern life leading to dangerous complications of atherosclerosis. Good control of indicators of dyslipidemia and atherosclerosis, including levels of triglycerides (TG), total cholesterol (TC), high-density lipoprotein cholesterol (HDL-C), low-density lipoprotein cholesterol (LDL-C) and very low-density lipoprotein cholesterol (VLDL-C), the atherogenic index (AI) contribute to preventing and reversing the progression of the disease.

The study aimed to evaluate the effect of regulating exogenous dyslipidemia of capsules prepared by the Vietnam Military Medical University containing fermented Allium sativum, Hibiscus sabdariffa, Gynostemma pentaphyllum and Alisma plantago aquatica on white rats. The recommended adult dose is 6 tablets/day, equivalent to 48 mg/kg/day. The dose conversion in rats (conversion factor is of 7) was 336 mg/kg/day. The reference drug was Atorvastatin, at dose of 10 mg/kg body weight of rats.

The results showed that, in the model batch of mixed cholesterol oil, the manifestations of dyslipidemia of rats were clearly shown through the increases of TG, TC, LDL-C, VLDL-C levels, and AI. There was a decrease in the above parameters and an increase in the concentration of HCL-C in the batch of research preparation and reference drugs.

The results of the study are promising for the use of this preparation in the treatment of dyslipidemia.

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# Transition metal (Co, Ni, Fe)-based materials - superior electrocatalyst for water splitting

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Nowadays, the increasing energy demand and environmental awareness have prompted extensive research on the development of alternative "green", "clean", "price competitive" energy conversion and storage technologies with high efficiency and low cost. Among them, water splitting is an attractive energy technology that has been concentrated by many researchers due to its excellent adaptability, generating hydrogen and oxygen through electrochemical energy. Water splitting comprises two half-reactions: hydrogen evolution reaction (HER) at the cathode and oxygen evolution reaction (OER) at the anode. However, it is well known that the state-of-the-art catalysts for HER and OER are Pt, Pt-based material, and IrO<sub>2</sub>/RuO<sub>2</sub>, respectively. Due to their price and scarcity, they are not suitable candidates for large-scale applications. Therefore, research and developing new electrocatalysts with high catalytic activity, optimal stability, and low cost are significantly concerned. Herein, in this present, we introduce the fabrication and development of transition metal (Co, Ni, Fe)-based electrocatalyst for water splitting with outstanding catalytic activity over broad pH ranges, long-term electrochemical durability, and competition with commercial catalytic materials.

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# Co-loading of nanosilver and nanoemulsion antibiotics plant-based *Allium sativum* extract in alginate/carboxyl methylcellulose carrier for antibacterial activity

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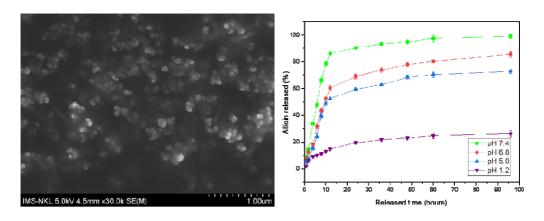
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Allium sativum is a medicinal herb that contains biologically active ingredients such as botanical antibiotic actives [1], but it has the disadvantage of being difficult to dissolve in lipids and difficult to absorb through biofilms in the gastrointestinal tract [2]. Nanosilver has long been used as a potential antibacterial agent, however, to achieve a bactericidal effect, high concentrations are required [3]. This leads to antibiotic resistance of microorganisms and environmental pollution [4].

In this work, to combine nanosilver to nanoemulsion antibiotics plant-based Allium sativum extract when using biocompatible scaffolds, we have established a solvent evaporative emulsification method to produce nanocarier of alginate/carboxyl methylcellulose. In which, silver nanoparticles were prepared by green method from aqueous extract of Allium sativum. The botanical antibiotic components of the alcoholic extract of garlic were emulsified with emulsifier poloxamer 407 to reduce the particle size, and make these active ingredients both water-soluble and lipid-soluble. The reaction mixture turned to yellow-brown color, transparent after 4 hours of incubation and exhibits an absorbance peak around 450 nm characteristic of Ag nanoparticle. Field emission Scanning electron microscopy and Energy-dispersive Xray analysis showed the prepared nanosystems were spherical shape, pure and polydispersed and the size was ranging from 50 to 100 nm. X-ray diffraction studies revealed that most of the nanoparticles were cubic in shape. Fourier transform infrared nanoparticles spectroscopy showed were capped with alginate/carboxyl methylcellulose carrier. In vitro drug release kinetics of Allicin from this nanosystem exhibited ability to release slowly compounds at different pH conditions which represent the biological environment of the body. This nanoformulation was compared for its antimicrobial activity against human pathogens (Staphylococcus aureus, Bacillus subtilis, Lactobacillus fermentum, Salmonella enterica, Escherichia coli, and Pseudomonas aeruginosa). Our results show that the nanosystem possess significantly higher antimicrobial activity against the tested organisms. Therefore, silver nanoparticles with plant antibiotics from garlic extracts were combined in the same nanosystem, it will increase the synergistic effect and the toxicity of nanosilver to healthy cells when used alone at high concentrations.



FESEM image and Drug release profiles of Allicin from nanoformulation

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## References

- [1] Strika I, Bašić A, Halilović N. Antimicrobial effects of garlic (Allium sativum L.). 17–20 (2016).
- [2] El-Saber Batiha G, Magdy Beshbishy A, G Wasef L, Elewa YHA, A Al-Sagan A, Abd El-Hack ME, Taha AE, M Abd-Elhakim Y, Prasad Devkota H. Chemical Constituents and Pharmacological Activities of Garlic (Allium sativum L.): A Review. *Nutrients*, **12**, 872 (2020).
- [3] Ferdous Z, Nemmar A. Health Impact of Silver Nanoparticles: A Review of the Biodistribution and Toxicity Following Various Routes of Exposure. *Int J Mol Sci*, **21**, 2375 (2020).
- [4] Panacek A, Kvitek L, Smékalová M, Večeřová R, Kolář M, Röderová M, Dycka F, Šebela M, Prucek R, Tomanec O, Zboril R. Bacterial resistance to silver nanoparticles and how to overcome it. *Nature Nanotechnology*, **13**, (2018).

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# Degradation of methyl blue by an approach using plasma jet processing

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Presently, the advantages of atmospheric pressure non-thermal plasma jet are developments and application in many different fields [1], especially the removal of harmful substances in water. Methyl blue is well - known colorant in diverse fields such as a chemical dye and harmful to human, animals and environmental [2,3], so its decomposition is necessary. In this study, we have set up an atmospheric pressure non-thermal plasma jet system to decompose Methyl blue. The combination of the UV / Vis analysis into the effectively investigation of voltage, Ar-gas speed, the  $\rm H_2O_2$  formation, the pH changes in the solution has supported to optimize the parameters of plasma jet system and clearly understand the mechanism in whole process. The result of our work shown the formation of  ${}^{\bullet}\rm{OH}$  – hydroxyl radical, a powerful oxidant leading to the directly entire degradation Methyl blue.

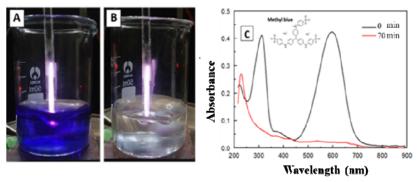


Figure 1: Methyl blue solution (A) Untreated; (B) Treated in 70 minutes by Plasma Jet; (C) Absorbance peak in 0 minute with 2 peaks at 600nm and 310nm and 70 minutes was degradation by plasma jet system

## References

- [1] R. Zhou, X. Wang, R. Zhou, J. Weerasinghe, T. Zhang, Y. Xin, H. Wang, P. Cullen, H. Wang, K.K.J.F.o.C.S. Ostrikov, Engineering, (2021) 1.
- [2] R. Suryavanshi, S. Mohite, A. Bagade, S. Shaikh, J. Thorat, K.J.M.R.B. Rajpure, 101 (2018) 324.
- [3] Y. Li, H. Lu, Y. Wang, Y. Zhao, X.J.J.o.M.S. Li, 54 (2019) 7603.

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# Determination of local anisotropy fields in polydispersed composites after FSP modification

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The local anisotropy in composites obtained as a result of Friction Stir Processing is investigated. The traces of inhomogeneity follow the trajectory of mechanical stirring, resulting in a local anisotropy [1,2]. This effect is invisible by means of direct observations and can be determined by combining of digital images processing from microscopic examination and of the theory of *Analytical Representative Volume Element* [1,3,4]. First, the local inhomogeneity is determined by estimation of the local particles concentration in the host medium by using image analysis. Then the initial anisotropy estimation is performed in the previously introduces value of the global anisotropy vector for monodispersed composites. The heterogeneus structures analyzed in this way allow for introduction of generalized anisotropy vector  $\kappa$  more suitable for complex study of polydispersed inhomogeneous composites.

The new value  $\kappa$  contains geometric informations which can also be obtained from the 2-point correlation functions.

Therefore, it properly describes the anisotropy of conductive fields in composites modeling thermal and electric conductivity, diffusion and elastic antiplane deformation

### References

- [1] P. Kurtyka, N. Rylko, *Quantitative analysis of the particles distributions in reinforced composites*, Composite Structures 182, 2017,
- [2] M. Stawiarz, P. Kurtyka, N. Rylko, S. Gluzman, *Influence of FSP process modification on selected properties of Al-Si-Cu/SiCp composite surface layer*, Composites Theory and Practice 19 (4), 2019,
- [3] S. Gluzman, V. Mityushev, W. Nawalaniec, *Computational Analysysof Structured Media*, Elsevier, 2017
- [4] V. Mityushev, Representative cell in mechanics of composites and generalized Eisenstein-Rayleigh sums, Complex Variables and Elliptic Equations 51 (2006)

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# Administrative reform below the Minh Menh dynasty (1820 - 1840)

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In May of the Nham Tuat year (1802), Nguyen Anh took the name Gia Long and in May of the Binh Dan year (1806),he was crowned Emperor at Thai Hoa Palace, Hue citadel. The Nguyen Dynasty was officially established. During his nearly 20 years of reign, Gia Long had introduced many policies and implemented many measures to consolidate and strengthen the country's unification. However, the administrative reform under Gia Long's reign had many corruptions, mandarins embezzlement, and tyranny raging at the intermediate and grassroots administrative levels. In the history of Vietnam's feudal system, the founding kings of the dynasty often set themselves the goal of "opening the door" rather than "defending the city", so they have more merit in martial arts than in literature. Therefore, the cause of literature and politics, including the reform of the country's administrative apparatus, was placed on the shoulders of the second king of the Nguyen Dynasty, Minh Menh. One of Minh Menh's political ideas was to consolidate national unity. Without a comprehensive reform of the administrative apparatus, it is impossible to speak of true national unity. The concept of national administrative reform is essentially the adjustment and renewal of the structure and operation of the management apparatus in terms of reorganization and institutional aspects to promote the effectiveness of the organization, to meet the requirements of objective reality, to quickly achieve the national development goals according to the authorities' consciousness. In order to restore the administrative reform process in the early 19th century and restore the appearance of the country's management apparatus under the reign of Minh Menh, in addition to relying on documents, letters, reports, monographs, and authorships. The author has relied on the principles of dialectical materialism and historical materialism in the study of history. In addition, the administrative reform from a structural point of view is the replacement of outdated and cumbersome elements and elements to reassemble into a more complete system. With the aim to highlight the work of "architect" Minh Menh in building the new administrative apparatus, we use the method of mapping the entire Central State Institution as well as the local state. In addition, to solve the problems posed in the article, we use the research method that synthesizes many scientific disciplines, in which the logical method combined with the historical method plays a key role. The article also uses specific methods of other sciences such as historical topography, statistics, etc. to support historical documents and to solve the problems posed by the article. The article has initially systematized and evaluated the documents as well as the research results on the administrative reform under the Minh Menh dynasty so far. Based on historical documents and other sources, the author tries to clarify and restore the administrative reform in particular and the state administrative apparatus from the central to local levels during the Minh Menh period. The article also initially provides the scientific basis to contribute with historians to review and reevaluate the position of the Nguyen Dynasty. The research shows that the

administrative reform that took place under the Minh Menh dynasty was one of the major administrative reforms in the history of the Middle Ages of Vietnam. From trying to clarify the deep and direct causes leading to that administrative reform and at the same time placing the reform in the contemporary historical context, the reform has brought into play the achievements of the Khuc and Le families. The positive side is the renewal and unification of the national administrative system, including the decentralization of the administrative system and the quotas and mandarin levels from the central to local levels, but it cannot solve the comprehensive crisis of the country. The decaying feudal society needed a transition to a higher socio-economic formincluding the Minh Menh Dynasty in the historical process of the nation. The research shows that the administrative reform that took place under the Minh Menh dynasty was one of the major administrative reforms in the history of the Middle Ages of Vietnam. From trying to clarify the deep and direct causes leading to that administrative reform and at the same time placing the reform in the contemporary historical context, the reform has brought into play the achievements of the Khuc and Le families. The positive side is the renewal and unification of the national administrative system, including the decentralization of the administrative system and the quotas and mandarin levels from the central to local levels, but it cannot solve the comprehensive crisis of the country. The decaying feudal society required a transition to a higher socio-economic form.

#### References

- 1. Dao Duy Anh, History of Vietnam From Origins to the End of the 19th Century, Hanoi, National Culture Publishing House. 2018.
- 2. Nguyen The Anh, Vietnam's economy and society under the Nguyen kings, Writers Association Publishing House 2018.
- 3. Tran Trong Kim, History of Vietnam, Culture and Information Publishing House, 2002.
- 4. Chesneaux (J), Contribution à l'histoire de la nation Vietnamienne, Editions Sociales, Paris, 1955.
- 5. Langlet (P), L'anciennehistoriographied'é tat au Vietnam, É'colefransaired'Extrême Orient, Tome I, Paris 1990.

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## Indo-Himalayan protected areas: mountain tourism

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The Himalayas are among the world's most popular mountaineering destinations for tourism. Millions of hikers, trekkers and climbers visit them. Sensitive to outside influences, the Himalayan environment of high mountain areas, until recently cut off from civilization, has been abruptly exposed to it. The Indian Himalayan region welcomes over 50 million tourists annually. Becoming a popular visitor destination, more and more protected areas (PAs) in the Himalayas have been opened to tourism. About 70% of the Himalayan mountain system is located within India. The Indian share of the range (396,405 km 2) contains 34,766 km 2 of PAs that account for 8.8% of the landmass. There is ongoing effort to preserve areas characterised by rare flora and fauna, where nature protection is on a par with commercial goals, that is tourism. The presentation will outline the state of the natural environment within PAs and the trends in the changes, implications on nature-based tourism (NBT) in the Indian Himalayan PAs and its challenges. The presenting author will also discuss the impact of tourism on local communities, and possible solutions to strengthen NBT management in mountainous PAs.

## References

- [1] Andrejczuk, W. (2016). *Himalaje: szkic fizyczno-geograficzny przyroda nieożywiona*. Acta Geographica Silesiana, 24, 5–28.
- [2] Apollo, M. (2015). The clash-social, environmental and economical changes in tourism destination areas caused by tourism the case of Himalayan villages (India and Nepal). Current Issues of Tourism Research, 5(1), 6–19.
- [3] Apollo, M. (2017a). The true accessibility of mountaineering: The case of the High Himalaya. Journal of Outdoor Recreation and Tourism, 17, 29–43.
- [4] Badola, R. (1998). Attitudes of local people towards conservation and alternatives to forest resources: a case study from the lower Himalayas. Biodiversity and Conservation 7, 1245–1259.
- [5] Gawlik, A., Apollo, M., Andreychouk, V., Wengel, Y. (2021). Pilgrimage tourism to sacred places of the high Himalaya. In D. Timothy & Eamp; G. Nyaupane (Eds), Tourism and Sustainable Development in the Himalayas: Social, Environmental, and Economic Encounters. New York: Routledge.
- [6] Zurick, D. & Dress of Kentucky. [2006]. *Ilustrated Atlas of the Himalaya. Lexington: The University*. Press of Kentucky.

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