The eighth Workshop of Vietnamese Students in Poland (WVSP2023)

Program and Abstracts

Warszawa, November 25-26, 2023

Warszawa

Information

“The eighth workshop of Vietnamese students in Poland” (WVSP2023) will be held on November 25-26, 2023. WVSP2023 is planned as a hybrid form (online and onsite) workshop at Warsaw. WVSP2023 is jointly organized by the Vietnam Association of Science and Technology in Poland, the Institute of Physics, Polish Academy of Science in Warsaw, and the Foundation for Supporting Integration of Vietnamese in Poland.

Workshop of Vietnamese Students in Poland has been organized every year since 2016. It is a forum for students, PhD students and young scientists to show their activities in the course of their studies and to present their obtained results in the scientific research. The scientific program of WVSP2023 will cover all domains of natural sciences, social sciences and technology (biology and medicine, physics and mathematics, information technology, humanities, social sciences and others). The participants of WVSP2023 will also have an opportunity to attend the special lectures concerned with the newest achievements in science and technology presented by the invited lecturers.

WVSP2023 will be also the opportunity for exchanging information and initiating collaborations. Thus, students, PhD students and young scientists, not only in Poland but also from other countries and especially from Vietnam, are welcome to participate and give the contribution to WVSP2023. The program of WVSP2023 is based on plenary lectures, invited talks, contributed talks and the poster session.

To encourage the participation of all participants, no fee is required. We could cover the cost of the meetings thanks to the financial support from the sponsors of Institute of Physics, Polish Academy of Sciences, Warsaw, Poland, Vietnam Association of Science and Technology in Poland, Association of Vietnamese in Poland "Solidarity and Friendship", Foundation for Supporting Integration of Vietnamese in Poland, and Vietnamese Business Association in Poland.

The workshop website is here:
http://info.ifpan.edu.pl/~masli/events/8thVietnamesestudentInPoland/index.html

Organizers and Committees

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Institute of Physics, Polish Academy of Sciences (PAS), Warsaw

Vietnam Association of Science and Technology in Poland

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13. **Marcin Nowotny**, *International Institute of Molecular and Cell Biology in Warsaw – IIMCB, Poland.*
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15. **Bartosz Rożycki**, *Institute of Physics, Polish Academy of Sciences, Warsaw, Poland*.
16. **Piotr Setny**, *University of Warsaw, Poland.*
17. **Nguyen Xuan Phuc**, *Institute of Materials Science, Vietnam Academy of Science and Technology, Hanoi, Vietnam.* (online)
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19. **Van Cao Long**, *Zielona Gora University, Poland.*
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35. **Dau Hong Quan**, *Department of Mathematics, Pedagogical University of Krakow, Poland*. (online)
36. **Hoang Thien Ly**, *Warsaw University of Technology, Poland*.
37. **Nguyen Cong Duc**, *Silesian University of Technology, Faculty of Civil Engineering, Department of Mechanics and Bridges, Gliwice, Poland*.
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67. **Thi Sinh Hoa Nguyen**, *Polish Japanese Academy of Information Technology, Poland*.

Program

First day, November 25th 2023

8:00-9:00 Registration

Chair: Mai Suan Li

9:00-9:15 Opening

9:15-9:55 **Marcin Nowotny**

International Institute of Molecular and Cell Biology in Warsaw – IIMCB, Poland

Cryo-electron Microscopy - A Revolution in Structural Biology That Helps Us Understand Life at the Atomic Level

9:55-10:20 **Nguyen Van Thai**

Vietnam Association of Science and Technology in Poland, Warsaw, Poland

How Polish Literature Is Widespread in Vietnam

10:20-10:45 **Piotr Setny**

University of Warsaw, Poland

Membrane Interactions and Fusion Thermodynamics of Influenza Virus Fusion Peptides

10:45-11:15 Coffee break and viewing of posters

Chair: Mateusz Chwastyk

11:15-11:40 **Bartosz Rożycki**

Institute of Physics, Polish Academy of Sciences, Warsaw, Poland

Membrane Curvature Sensing by Model Biomolecular Condensates

11:40-11:52 **Nguyen Truong Co**

Department of Theoretical Chemistry, Gdansk University, Poland

Understanding Protein Self-Assembly in Varied Environments Through Lattice modeling

11:52-12:04 **Izabela Siekierska,** *Centre of New Technologies, University of Warsaw, Poland*

Peptide nucleic acid conjugates with membrane-active peptides and their stapled analogs as antimicrobial agents

12:04-12:16 **Panagiotis Theodorakis**, *Institute of Physics Polish Academy of Sciences, Warsaw, Poland*

Durotaxis and Antidurotaxis Motion onto Gradient Brush Substrates

12:16-12:28 **Luis H. Carnevale**, *Institute of Physics Polish Academy of Sciences, Warsaw, Poland*

Thermal Fluctuation break-up of Surfactant-Laden Liquid Threads

12:28-14:00 Lunch

Chair: Hoa K. N. Nhu-Tarnawska

14:00-14:40 **Tomasz Story**, *Institute of Physics, Polish Academy of Sciences, Warsaw, Poland.*

Topological Matter

14:40-15:05 **Andrzej Kozłowski**, *AGH University of Science and Technology, Krakow, Poland.*

The Magnetite Stone

15:05-15:30 **Hung Tan Pham**, *Department of Chemistry - KU Leuven, Belgium*

Mechanism of Glucose Electrooxidation to Gluconolactone on Gold Nanocluster Surface

15:30-15:42 **Soheil Arbabi**, *Institute of Physics, Polish Academy of Sciences, Warsaw, Poland*

Molecular Dynamics Simulation of the Coalescence of Droplets

15:42-16:05 Coffee break and viewing of posters

Chair: Bartosz Rożycki

16:05-16:30 **Piotr Szymczak**, *University of Warsaw, Poland*

Knotted Loops Fall Flat

16:30-16:42 **Hui Liu**, *Institute of Physics, Polish Academy of Sciences, Warsaw, Poland*

Kink-Meson Inelastic Scattering

16:42-16:54 **Hoang Thien Ly**, *Warsaw University of Technology, Poland*

Empirical Validation of Graph Structure Learning for Citation Network Applications

16:54-16:06 **Thang Do**, *Faculty of Geology, University of Warsaw, Poland*

New study on the age of Tertiary sediments in the Na Duong Basin (Northern Vietnam) based on palynological analysis

16:06-17:18 **Mai Van Hai**, *Department of Scientific management, Institute of Psychology, Vietnam Academy of Social Sciences, Vietnam*

The Interdependence of Happiness and Filial Piety Within the Family – A Study in Vietnam

17:18-17:30 **Kieu Kim Anh**, *Faculty of Journalism, Information and Book Studies, University of Warsaw*

Strategic Enhancement of Vietnam's Red River Delta Primary School Libraries

19:00-21:00 Banquet

Second day, November 26th 2023

Online talks

Chair: Mai Suan Li

9:00-9:15 **Young Research Award Lecture**

Ngan Le, *Institute of Astronomy, Nicolaus Copernicus University in Toruń, Poland*.

Impact of Metallicity on Far-infrared Line Cooling in the Embedded Cluster Gy 3-7 in the Outer Galaxy

9:15-9:40 **Nguyen Xuan Phuc**, *Institute of Materials Science, Vietnam Academy of Science and Technology, Hanoi, Vietnam*

Electromagnetic Heating Using of Nanomaterials and Its Applications

Chair: Panagiotis Theodorakis

9:40-9:52 **Nguyen Thi Thu Trang**, *AGH University of Krakow, Kraków, Poland*

Study of the thermomechanical behavior of S355 steel at extra high temperatures using the Gleeble system

9:52-10:04 **Thi Thu Ha Nguyen**, *University of the National Education Commission, Kraków, Poland*

DFT study of structural and electronic properties of double perovskites Ba_2MnWO_6 and Ba_2TiMnO_6

10:04-10:16 **Thi Hong Quan Vu**, *Insitute of Low Temperature and Structure Research, Polish Academy of Sciences, Wrocław, Poland*

Effect of A-site cation substitution in A_2MgWO_6 double perovskites doped with Dy_{3+} (A = Ca, Sr, Ba) on the crystal structure, luminescence and temperature sensing performance

10:16-10:28 **Dau Hong Quan**, *Department of Mathematics, Pedagogical University of Krakow, Poland*

Fixed Points of Monotone Operators Via Measure of Noncompactness

10:28-10:40 **Nguyen Thi Thu Thuy**, *Ho Chi Minh City University of Culture, Ho Chi Minh city, Vietnam*

Researching the impact of Korean popular culture on students' cultural practices in Ho Chi Minh City

10:40-10:52 **Nguyen Van Chung**, *Quang Binh University, Vietnam*

Factors Affecting Digital Transformation in Tourism Human Resource Training: Case Study of Central Coastal Provinces

Online talks end

10:52-11:32 **Hung Son Nguyen**, *University of Warsaw, Poland*

Generative AI in Education Learning and Teaching

11:32 -12:00 Coffee break and viewing of posters

Chair: Piotr Setny

12:00-12:25 **Van Cao Long**, *Zielona Gora University, Poland*

Quantum Optics and the Last Two Nobel Prizes

12:25-12:37 **Pamela Smardz**, *Institute of Physics Polish Academy of Sciences, Warsaw, Poland*

Exploring Disulfide-Bond Functions in Proteins through Molecular Dynamics Simulations

12:37-12:49 **Julia Macyszyn**, *Centre of New Technologies, University of Warsaw, Warsaw, Poland*

Hydrocarbon stapling to initiate the antibacterial activity of a cell-penetrating peptide $(KFF)_3K$

12:49-13:01 **Monika Wojciechowska**, *Centre of New Technologies, University of Warsaw, Warsaw, Poland*

Stapled anoplins - in search of a drug for pathogens

Chair: Van Cao Long

13:01-13:13 **Nguyen Cong Duc**, *Silesian University of Technology, Faculty of Civil Engineering, Department of Mechanics and Bridges, Gliwice, Poland*

The Internet of Bridge Things: A Reviewing of AI-assisted Structural Health Diagnostic

13:13-13:40 **Phong Ba Dao**, *AGH University of Krakow, Poland*

On Wilcoxon Rank Sum Test for Condition Monitoring and Fault Detection of Wind Turbines

13:40-13:50 Closing

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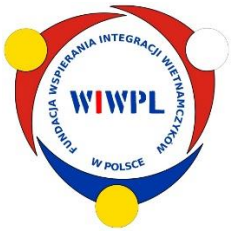

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PLENARY LECTURES

Generative AI in Education Learning and Teaching

Hung Son Nguyen[1]

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Abstract

Generative AI (GenAI) refers to AI techniques that learn a representation of artifacts from data and use it to generate unique content (including images, video, music, speech, and text) that preserves a likeness to original data.

The increased adoption of GenAI tools, like ChatGPT developed by OpenAI, and Bard, an AI experiment by Google, creates opportunities for its use in academic research, knowledge development, and AI-assisted authoring. Integrating AI into higher education is not a futuristic vision but an inevitability. This talk highlights this trend, discussing the implications of generative AI use in education and actions the colleges and universities must adapt and prepare students, faculty, and staff for their AI-infused futures.

Schools and universities are generally slow to adapt to change. In the recent past, other technology tools have been met with consternation in schools. For example, the use of calculators in the classroom was banned, and Wikipedia was considered an unreliable source that should be avoided. And while calculators and Wikipedia may not be fully integrated into every classroom, they don't attract as much ire as they did in the past. Generative AI is different from these innovations. Artificial intelligence is not a device that can be banned, it is not a source that students can be instructed not to use, and its use cannot be detected by primitive plagiarism tools. This new technology will be hard to avoid. Generative AI integration may become so pervasive and so quickly that students may not even realize they are using the tools they are using.

While there are many issues surrounding GenAI, such as ethical concerns, copyright and intellectual property questions, and biases within the training data, we will focus only on the integration of GenAI into higher education teaching and learning.

There is a duality of AI on many college campuses. On the one hand, some education officials welcome AI tools to help recruit and enroll students, but on the other hand, many faculty and other university staff believe that the use of GenAI is a form of fraud or a breach of academic integrity. What is more ethical: directing the use of AI tools or pretending they don't exist?

Ignoring GenAI or banning its use in the academic part of higher education seems naive and probably wrong. Shouldn't universities be preparing graduates to work in a world where GenAI is becoming ubiquitous?

In its regulations, UNESCO recommended that member states "work with international organizations, educational institutions, and private and non-governmental entities to provide adequate

AI literacy education to the public on all levels in all countries in order to empower people and reduce the digital divides and digital access inequalities resulting from the wide adoption of AI systems". We will analyze how countries such as the USA, Singapore, South Korea, India, China, Finland, Japan or the European Union are implementing these UNESCO recommendations.

References

[1] Anna Teichmann. Guidance for generative AI in education and research. https://epale.ec.europa.eu/en/resource-centre/content/guidance-generative-ai-education-and-research.

[2] Guidance for generative AI in education and research https://www.unesco.org/en/articles/guidance-generative-ai-education- and-research.

[3] Shockwaves & Innovations: How Nations Worldwide Are Dealing with AI in Education https://www.ntu.edu.sg/nie/news-events/news/detail/shockwaves-innovations-how-nations-worldwide- are-dealing-with-ai-in-education.

Cryo-electron Microscopy - A Revolution in Structural Biology That Helps Us Understand Life at the Atomic Level

Marcin Nowotny[1]

[1]*Laboratory of Protein Structure, International Institute of Molecular and Cell Biology; 02-109 Warsaw, Poland*

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Abstract

Structural biology aims to visualise biological molecules, in particular proteins and nucleic acids, at the level of individual atoms. For a long time it was dominated by protein crystallography, but recently cryo-electron microscopy (cryo-EM) has become the method of choice for structural studies. Electron microscopy is an old technique, but it is only in the last decade or so that technical developments have enabled it to provide structural information of similar quality to crystallography. This has led to a real revolution in our understanding of complex biological molecular machines. I will discuss the basics of cryo-EM and in particular the recent technical advances.

I will also describe our recent studies using cryo-EM, in particular on AbiK, an unusual bacterial DNA polymerase involved in phage defence. It is a very unique enzyme because it can synthesise long stretches of single-stranded DNA without the need for a template or primer. For priming, it attaches the first nucleotide to its own tyrosine residue. I will also present our cryo-EM structural data for a complex of RecF-RecR-RecO proteins involved in bacterial homologous recombination - one of the major DNA repair pathways. Understanding the mechanism of this fascinating machinery has only been possible thanks to cryo-EM structure determination.

Topological Matter

Tomasz Story[1,2]

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[2]*International Research Centre MagTop, Institute of Physics PAS, Warszawa*

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Abstract

Several families of semiconductors known for infrared or thermoelectric applications, such as mercury-, bismuth-, antimony- or tin-chalcogenides, are materials platform for experimental and theoretical development of new condensed matter electronic systems that constitute the, so called, topological matter. Nowadays, it covers topological insulators, topological Weyl or Dirac semimetals, topological superconductors as well as Quantum Hall systems. These materials exhibit surface (2D) or edge (1D) conduction with unusual properties driven by strong relativistic (spin-orbital) effects. In the bulk they exhibit inverted ordering of valence and conduction bands while at the boundaries (surfaces, edges) they reveal metallic in-gap states of linear (Dirac-like) electron energy dispersion and strong spin-momentum locking.

I will show how unique possibilities of controlling electronic structure as well as electric, optical or magnetic properties of semiconductors can be used to experimentally study the surface or edge topological states by angle- and spin-resolved photoemission, scanning tunneling spectroscopy and magneto-transport or magneto-optical effects.

Experimental realization of these ideas and testing various applicational concepts (like topological transistors, topological qubits or topological spin current sources) requires topological materials in the form of highest quality bulk crystals, layered heterostructures or nanowires of various semiconductors, semimetals and superconductors.

I will also show that apart of electronic solid state systems, topological classification applies to other, both quantum and classical, physical systems, like photonic, magnonic or vibrational structures, thus uncovering the intriguing new features at their boundaries.

References

[1] P. Dziawa, B.J. Kowalski, K. Dybko et al., Nature Mat. **11**, 1023 (2012).

[2] P. Sessi, D. Di Sante, A. Szczerbakow et al., Science **354**, 1269 (2016).

[3] K. Dybko, M. Szot, A. Szczerbakow et al., Phys. Rev. B **96**, 205129 (2017).

[4] A. Łusakowski, P. Bogusławski, and T. Story, Phys. Rev. B **103,** 045202 (2021).

[5] J. Jung, A. Odobesko, R. Boshuis et al., Phys. Rev. Lett. **126**, 236402 (2021).

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[7] G.. Wagner, S. Das, J. Jung et al., Nano Lett. **23**, 2476 (2023).

INVITED TALKS

Membrane Curvature Sensing by Model Biomolecular Condensates

Midhun Mohan Anila[1], Rikhia Ghosh[2], Bartosz Różycki[1]

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Abstract

Biomolecular condensates (BCs) are fluid droplets that form in biological cells by liquid-liquid phase separation. Their major components are intrinsically disordered proteins. Vast attention has been given in recent years to BCs inside the cytosol and nucleus. BCs at the cell membrane have not been studied to the same extent so far. However, recent studies provide increasingly more examples of interfaces between BCs and membranes which function as platforms for diverse biomolecular processes. Galectin-3, for example, is known to mediate clathrin-independent endocytosis and has been recently shown to undergo liquid-liquid phase separation, but the function of BCs of galectin-3 in endocytic pit formation is unknown. Here, we use dissipative particle dynamics simulations to study a generic coarse-grained model for BCs interacting with lipid membranes. In analogy to galectin-3, we consider polymers comprising two segments – one of them mediates multivalent attractive interactions between the polymers, and the other one has affinity for association with specific lipid head groups. When these polymers are brought into contact with a multi-component membrane, they spontaneously assemble into droplets and, simultaneously, induce lateral separation of lipids within the membrane. Interestingly, we find that if the membrane is bent, the polymer droplets localize at membrane regions curved inward. Although the polymers have no particular shape or intrinsic curvature, they appear to sense membrane curvature when clustered at the membrane. Our results indicate toward a generic mechanism of membrane curvature sensing by BCs involved in such processes as endocytosis.

References

[1] Midhun Mohan Anila, Rikhia Ghosh, Bartosz Różycki (2023). *Membrane curvature sensing by model biomolecular condensates*. Soft Matter 19(20): 3723-3732.

Membrane Interactions and Fusion Thermodynamics of Influenza Virus Fusion Peptides

Piotr Setny[1]

[1]*University of Warsaw, Poland*

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Abstract

Influenza viruses enter cells by fusing their lipid envelopes with host membranes. Directly responsible for membrane merger are N-terminal fragments of hemagglutinin (HA) subunit 2, so called fusion peptides (HAfps). It has long been known that isolated HAfps, merely 23 amino acids long, can fuse liposomes on their own, without the aid of the entire HA protein. Despite years of studies, however, the details of their interaction with the target membrane and the actual mechanism of fusogenic action remain elusive.

I will present insights obtained from series of atomistic molecular dynamics simulations directed at capturing HAfps conformational equilibria, localization within the membrane, mutual interactions, and thermodynamic effect on membrane fusion. The results indicate that, aside from widely acknowledged peptides binding to membrane surface, there is also a possibility of them adopting a transmembrane configuration. This configuration, being only metastable in the case of isolated HAfps, is significantly enhanced by peptides trimerization, which mirrors their native multimeric state. By calculating fully atomistic potentials of mean force for membrane stalk formation I will demonstrate that both, the surface and deeply bound peptide configurations are actually capable of lowering the free energy barrier for the first fusion intermediate. This observation points to two plausible, peptide-driven fusion mechanisms. The first one, involving transmembrane bound HAfp, relies on the creation of, so called, stalk-hole complex. The second, mediated by surface bound HAfp proceeds owing to peptide's ability to stabilise stalk by snuggly fitting into the region of extreme negative membrane curvature. The relevance of the above findings in the light of experimental data will be discussed.

Electromagnetic Heating Using of Nanomaterials and Its Applications

Nguyen Xuan Phuc[1]

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Abstract

This review [1] will introduce general theoretical and experimental aspects of the alternating electric field (AEF) and magnetic field (AMF) stimulated heating on nanomaterials. Attempts to fabricate magnetic nanoparticles (MNPs) and photothermal nanoparticles (PNPs) of improved heating efficiencies will be reviewed and those with the highest specific loss power have been summarized. Finally, potential applications, including cancer treatment using AMF@MNP hyperthermia and AEF@PNP hyperthermia, AMF@MNP and AEF@PNP triggered drug release, as well as nanocomposite processing will be particularly highlighted. Besides, other exotic applications such as toxic solvent desorption from adsorbent materials, thermophoresis in precise membrane melting as well as optical signal processing in heat-assisted magnetic memory technology will be also outlined. The various applications will be attempted to represent into 2 groups: biomedicine and materials processing, which are composed of localized/targeted and volumetric heating type.

References

[2] Nguyen Xuan Phuc, Do Hung Manh, Pham Hong Nam, Vietnam Journal of Science and Technology 61(2) (2023) 137-164.

Mechanism of Glucose Electrooxidation to Gluconolactone on Gold Nanocluster Surface

Hung Tan Pham[1], Daniel Escudero Masa[*,1]

[1]*Department of Chemistry, KU Leuven, Celestijnenlaan 200F 3001 heverlee, Leuven, Belgium*

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Abstract

We develop a computational workflow for high – throughput screening of nanocluster catalyst for glucose oxidation. Our approach evaluates electrocatalytic performance of nanoclusters at thermodynamic and kinetic viewpoints. The workflow begins with randomly generating a huge number of initial conformers, then performs a massive geometry optimization to find the stable conformers of glucose on nanocluster surface. A python module is built to construct the free energy diagram based on the computational hydrogen electrode method (CHE) potential. In combination with xTB package, this module generates automatically intermediates from the stable conformers, and performs geometry optimization. We use transition state optimization of Gaussian package to find TS. Herein we present the detailed mechanism of glucose oxidation on Au_{147} nanocluster using our computational workflow.

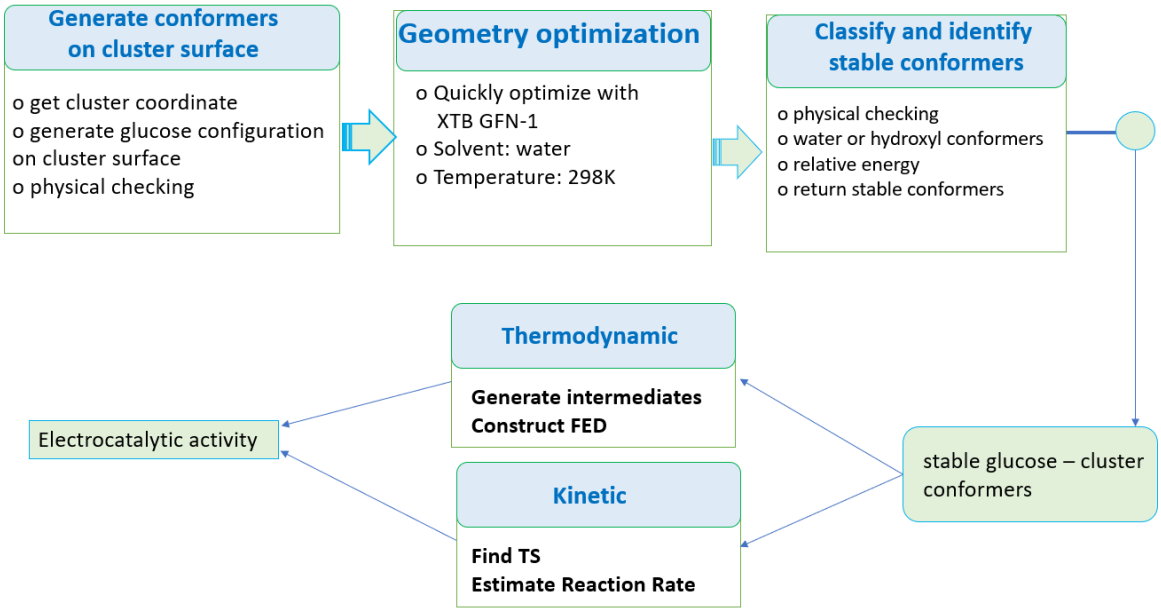

Figure caption: computational workflow for high – throughput screening of nanocluster catalyst for glucose oxidation.

Knotted Loops Fall Flat

Magdalena Gruziel, Krishnan Thyagarajan, Giovanni Dietler, Andrzej Stasiak, Maria Ekiel-Jeżewska, and Piotr Szymczak

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Abstract

Long-chain molecules, like DNA, can develop knots, and these knots in turn affect how the molecules move through a liquid. To understand this behavior, together with a Giovanni Dietler group from EPFL Lausanne we have devised an experiment with knotted loops made of steel beaded chain. Surprisingly, all the loops settled into horizontally flat configurations as they fell—no matter how they were initially dropped. The loops in this configuration perform a highly concerted motion, which is a superposition of downward translation, rotation of the individual strands around each other and much slower rotation of the entire structure around the vertical axis. Interestingly, a very similar motion has been reported previously in a completely different context of knotted vortices in an ideal fluid. We then study this motion in a more detail using Stokesian Dynamics simulations of a flexible chain represented in terms of the bead-and-spring model.

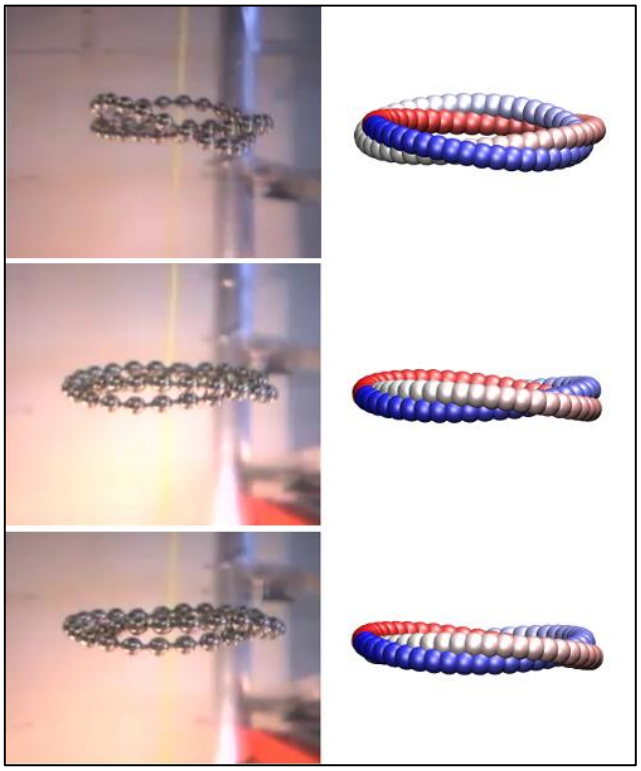

Figure caption: Knotted loops settling in a viscous fluid: experiment (left) and computer simulation (right).

We also consider the sedimentation of unknotted loops and show that at relatively small bending stiffness, a rich zoology of periodic orbits and stationary states appear, including double and triple loops, rotating figure-of-eight, swinging periodic motions or tank-treading solutions. These solutions are characterized by different sedimentation velocities, which can be used to differentiate them experimentally.

These results are important not only for elucidating the link between topology and dynamics of filamentous objects but also for understanding of the appearance of periodic solutions in the sedimentation of many-particle systems in a viscous fluid.

The Magnetite Stone

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Abstract

This presentation is intended for a general audience. I will present the history of the discovery of magnetite and the role it played as a mysterious object in antiquity and the Middle Ages. The increasing role of magnetite as the object of the earliest known European experimental scientific work will also be presented. I will briefly describe the phenomenon of magnetism and the way in which magnetite, as a magnetic natural mineral, is exploited. I will then describe the other interesting phenomenon in magnetite, the Verwey phase transformation. This will be followed by a description of three experiments, and the results of these experiments, which have been used to study and understand this phase transition. I will conclude my talk by saying that magnetite has now become a model system in which all the typical solid state interactions are present and accentuated.

Quantum Optics and the Last Two Nobel Prizes

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Abstract

The speech briefly presented the history on research of light and the two most recent Nobel Prizes in physics related: Entanglement effect and teleportation (Nobel Physics 2022), creating extremely short attosecond pulses for creating possibility for observation of very fast dynamics as dynamics of electrons in atoms and the electron motion in photoelectric effect (Nobel Physics 2023). This is the result of research in the field of quantum optics, the first doctoral thesis in Poland in quantum optics was formed in 1979 (Cao Long Van), in which the photon discovered by Einstein in 1905 plays a key role.

How Polish Literature Is Widespread in Vietnam

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Abstract

Polish literature has been known to the Vietnamese since the mid-1950s. In 1955, they published the book "Adam Mickiewicz, the great poet of Poland and the world" to commemorate the hundredth anniversary of Mickiewicz's death. Later they published "Anthology of Polish poetry". The authors of the translations of the poems were famous Vietnamese poets TE HANH and NGUYEN XUAN SANH. An interesting phenomenon was that in 1969, in South Vietnam, a country that was not friendly with Poland at that time, Sławomir Mrożek's short story "The Elephant" was published.

While before 1975 Polish literature was translated into Vietnamese mostly using a third language, mainly French and Russian, since the 1980s direct translations have dominated. A real event in the popularization of Polish literature in Vietnam was the publication in 1985 of Quo Vadis, the masterpiece of the Polish Nobel Prize winner Henryk Sienkiewicz, translated by NGUYEN HUU DUNG. This event marked the beginning of the golden age of Polish literature in Vietnam. So far, they have published over 100 Polish books translated into our language.

NGUYEN HUU DUNG stayed in Poland in the 1970s as a PhD student in technical sciences. After returning to Vietnam, he worked in the field of fisheries and marine products, but he loved Polish literature and translated many Polish books, such as In Desert and Wilderness by Henryk Sienkiewicz, The Career of Nikodem Dyzma, The Quack and Professor Wilczuk by Tadeusz Dołęga-Mostowicz, The Leper by Helena Mniszkówna. In 2022, he published "Teutonic Knights" by Henryk Sienkiewicz. In total, he has over 10 translated books.

LE BA THU graduated from the Faculty of Geodesy and Cartography of the Warsaw University of Technology. For 25 years he worked as a translator at the Polish embassy in Hanoi, then he was the first secretary of the Vietnamese embassy in Poland. He translated over 20 Polish books, including: Pharaoh by Bolesław Prus and other modern Polish authors.

TA MINH CHAU, graduate of the Faculty of Philology at the University of Warsaw, former Vietnamese ambassador to Poland and Laos, specializes in translating poems, e.g. Selected poems by Wisława Szymborska (published in 1997, shortly after the author was awarded the Nobel Prize), selected poems by Czesław Miłosz.

NGUYEN CHI THUAT, a graduate of a Polish university, was a professor at the Adam Mickiewicz University in Poznań and a long-time Polish language teacher at the University of Hanoi. He has over 15 translated books, including: Bolesław Prus's Laka, Ryszard Kapuściński's Emperor.

NGUYEN THI THANH THU, a graduate of the Wrocław University of Science and Technology, has

over 15 translated books. Solitude on the Internet by Janusz Leon Wiśniewski has been reprinted 10 times.

NGUYEN THAI LINH, graduate of the Faculty of Law of the University of Warsaw, translated mainly Ryszard Kapuściński: Travels with Herodotus and Herban., as well as poems by Szymborska.

NGUYEN VAN THAI, graduate of the Warsaw University of Technology, is a habilitated doctor in geodesy. He translated, among others, Pan Tadeusz by Adam Mickiewicz, Chłopów by Władysław Reymont, Polish Novellas (by Sienkiewicz, Prus, Żeromski, Orzeszkowa, Konopnicka), Hania, In the desert and in the wilderness by Henryk Sienkiewicz, Bieguni by Olga Tokarczuk.

On Wilcoxon Rank Sum Test for Condition Monitoring and Fault Detection of Wind Turbines

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Abstract

Predictive maintenance has been considered as an effective strategy to reduce operations and maintenance (O&M) costs and improve the availability and efficiency of wind turbines through condition monitoring (CM) and fault detection, prediction and diagnosis. Wind turbine monitoring using data collected by the supervisory control and data acquisition (SCADA) systems has been seen as a cost-effective and wide-scale approach. As a result, much research has employed SCADA data to develop reliable, efficient and cost-effective monitoring systems in recent years. Most solutions are based on statistical methods and machine learning (ML) techniques. However, these existing approaches face two major challenges.

The first major challenge involves a common practice of the statistical and ML-based methods regarding the use of normal behaviour models (NBMs) developed for specific turbine components. NBMs are based on the idea of modelling the normal behaviour of critical components using historical SCADA data collected while the wind turbine was operating in healthy condition. Then, the detection of faults are based on the analysis of deviations between the predicted model outputs and actual measured values. However, since each wind turbine has many critical components that need to be monitored, NBM-based approach would require users to build and preserve a large number of NBMs for any wind farm. Moreover, due to many unavoidable reasons, e.g. wind turbine ageing, subsystem replacements, software updates, or sensor recalibration, NBMs are supposed to vary with time. Hence, one would raise many concerns about the updating issues of NBMs, e.g. when or how often a model should be updated to assure the homogeneity between the model and the turbine subsystem. These problems lead to the circumstance that it is not easy for wind farm operators to make use of this monitoring approach.

The second major challenge relates to the fact that many statistical approaches for wind turbine condition monitoring were developed on the basis of parametric models. In addition, it is argued that deep learning models can generally be viewed as parametric methods. When using parametric statistical models, it is often assumed that the analysed SCADA data follow a normal distribution. However, if the data are not normally distributed and not transformed to approximate to a normal distribution, the use of parametric approaches to build NBMs might not be appropriate and could diminish the fault detection process.

The present study aims to close this gap by introducing a nonparametric statistical approach to wind turbine condition monitoring. Specifically, the Wilcoxon rank sum test, a nonparametric statistical test method in the field of statistics, which was proposed by Frank Wilcoxon in 1945 [1], has been adapted for the operation state monitoring and automatic fault detection of wind turbines. The test is often used to determine whether two independent or unpaired groups of populations (data sets) are statistically different. Samples from two groups can be of different lengths. This test is equivalent to the Mann-Whitney U-test [2]. The Wilcoxon rank sum test is known as a nonparametric alternative to the conventional two-sample Student's t-test (a popular parametric statistical test).

Based on the Wilcoxon rank sum test, a five-step computation procedure has been developed in which the fault detection process is relied on statistical hypothesis tests. The null hypothesis is defined as that the wind turbine is operating in the normal condition without fault. If the null hypothesis is rejected in favour of the alternative, this indicates the occurrence of a fault in the wind turbine. The detection of a fault is indicated by an abrupt change from 0 to 1 in the test decision. The method can monitor one or several key process parameters of the wind turbine simultaneously. The monitoring process for each process parameter uses only its own data, thus, is independent with the monitoring process for other parameters. Hence, we do not need to handle the correlation between the selected parameters. Two wind turbine SCADA data sets, including three fault events, were used as case studies for testing the developed method. In both cases, various process parameters were analysed. The results show that the method can effectively monitor the operation state of wind turbines and reliably detect the anomaly (or fault) several days before its occurrence.

For further descriptions of the developed method as well as the testing results obtained, potential readers are refferred to the paper [3] published recently in Applied Energy.

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CONTRIBUTED TALKS

Understanding Protein Self-Assembly in Varied Environments Through Lattice Modeling

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Abstract

This talk presents a lattice model analysis of polypeptide chain self-assembly into fibrils, a key process in neurodegenerative diseases. We investigate how crowding agents and surface roughness affect fibrillation kinetics. Our findings indicate that larger crowders decrease the fibril formation time (τ fib), while smaller crowders increase it, suggesting an optimal crowder size for accelerated fibrillation. This behavior is explained by the competing energetic and entropic factors, with τfib exhibiting a parabolic response to confinement size. Additionally, we demonstrate that increased surface roughness slows fibrillation, but moderately rough surfaces can subtly catalyze polypeptide assembly without delay, balancing energy and entropy interactions. These insights highlight the intricate nature of protein self-assembly in complex environments, providing valuable information for potential treatments of amyloid-related diseases.

Thermal Fluctuation break-up of Surfactant-Laden Liquid Threads

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Abstract

Formation of droplets is a fundamental process used in many industrial applications, such as inkjet printing and drug manufacturing. The break-up of a liquid thread is influenced by an instability dependant on surface tension. We can reduce the surface tension by adding surfactants, which are molecules that adsorb on the interface of liquids, and thus, change the break-up dynamics. At certain systems with ultra-low surface tension or very small length scales, thermal fluctuations on the interface are capable of creating the instability that leads to the formation of droplets and satellite droplets. In our study, we employ simulations of a coarse-grained model to determine the characteristic wavelength of such instabilities on liquid nanothreads with various surfactant concentrations, above and below its critical aggregation concentration. Also, we have identified the different break-up regimes and their time-scales. We anticipate that our study contributes to the understanding of a fundamental process in nature and paves the way for further developments in this area for relevant applications.

** This research has been supported by the National Science Centre, Poland, under Grant No. 2019/34/E/ST3/00232. We gratefully acknowledge Polish high-performance computing infrastructure PLGrid (HPC Centers: ACK Cyfronet AGH) for providing computer facilities and support within computational Grant No. PLG/2022/015261.*

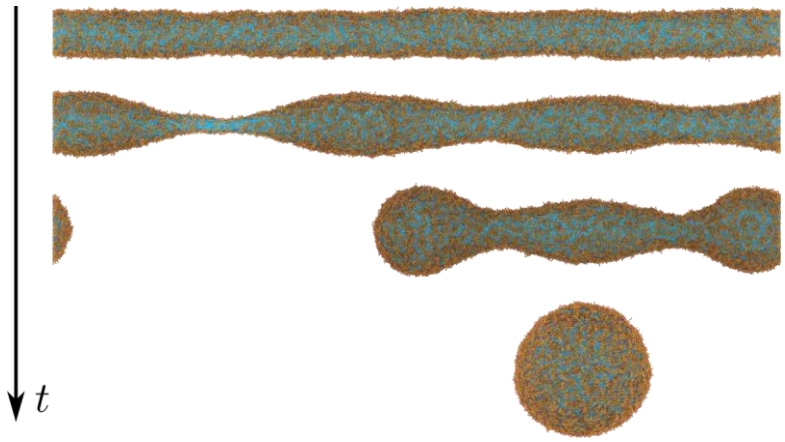

Figure caption: Simulation snapshots of the break-up of a surfactant laden liquid thread forming a droplet.

Study of the Thermomechanical Behavior of S355 Steel at Extra High Temperatures Using the Gleeble System

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Abstract

This study used the Gleeble System, to subject steel samples to a controlled high-temperature environment. Advanced equipment, including thermocouples and high-speed cameras, provide real-time data collection and analysis. The research process has established experiments for resistance heating and deformation processes of steel samples [1]. This allows precise determination of temperature, strain rate, and mechanical load, allowing detailed analysis of the steel's response to various thermal and mechanical stresses.

Research results have clarified the influence of temperature on the mechanical properties of steel. The findings of this study have far-reaching implications for industries that depend on high-temperature steel applications. Furthermore, the obtained results contribute to the development of advanced steel alloys suitable for specific applications, helping to improve efficiency, durability, and safety in industrial processes at extra-high temperatures.

Research equipment and materials

The Gleeble system

The Gleeble thermomechanical simulator reproduces on small samples the changes in temperature, stress, and deformation of the material under conditions similar to the actual manufacturing process [2]. Additionally, its vacuum chamber ensures a stable, contamination-free, and controlled environment for testing materials to obtain accurate and reliable data on material behavior (Fig 1a).

Material for study

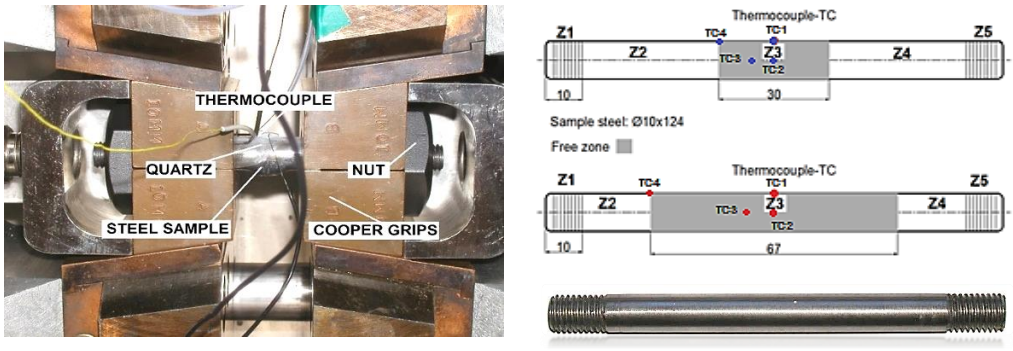
In this study, experiments were performed using the flexible testing capabilities of the Gleeble 3800 thermomechanical simulator. Steel grade S355 was used, its main chemical composition is given in Table 1 [3].

The cylindrical test specimen has a diameter of Ø10 mm and a length of 124 mm. The test patterns used include the position of the thermocouple (TC) and the position of the heat transfer zone, the free zone, designated Z1 to Z5. Zones Z1, Z3, Z5 are zones that transfer heat freely to the environment. Regions Z2 and Z4 are the contact areas of the sample with the position of the thermocouple (Fig. 1b).

Table 1. The chemical composition of the sample tested steel S355 (%)

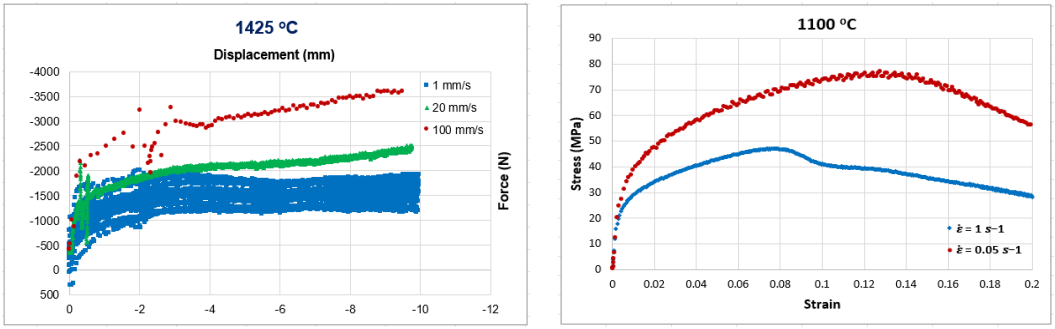
Steel (%)	C	Mn	Si	P	S	Cr	Ni	Al
S355	0,16	1,26	0,26	0,011	0,009	0,14	0,06	0,025

Experiments on the resistance heating process, compression, and tensile deformation processes recorded the current values and temperature values at the locations of different thermocouples on the test sample, showing that there exists a non-uniform temperature gradient. At the same time, the applied force value and strain stress value are also recorded very specifically and clearly, corresponding to each deformation rate of 0.05 s^{-1} and 1 s^{-1} (Fig 2a,b). All of these values significantly affect the properties of the material and have a strong impact on the deformation process of the test sample.



a) b)

Figure 1: The experimental equipment of the Gleeble 3800 system (a), Schematic and image of steel sample with the position of the thermocouple (b) ("cold" grips-blue, and "hot" grips-red).



a) b)

Figure 2: Compression force and displacement curves of the tests at 1425 °C with velocities of 1, 20, and 100 mm/s (a); stress-strain curves of the tests at 1100 °C, deformation rate of 0.05 s^{-1} and 1 s^{-1} (b).

In summary, this work aims to gain a deeper understanding of how steel behaves under extremely high temperatures and mechanical stress during deformation. This knowledge could have important implications for various industries, leading to the development of more robust and efficient materials and manufacturing processes.

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Exploring Disulfide-Bond Functions in Proteins through Molecular Dynamics Simulations

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Abstract

Proteins play a pivotal role in the functioning of living organisms. Their versatile functions encompass acting as catalysts, providing structural support to cells and tissues, facilitating molecular transport, regulating biological processes through signaling and gene expression, and contributing to the immune system's defense mechanisms. To perform their functions effectively, many proteins must achieve the correct structure, and knowledge of their structural organization is essential for understanding their biological role. In addition to experimental techniques such as X-ray crystallography, Nuclear Magnetic Resonance (NMR), and cryo-Electron Microscopy (cryo-EM) used for structural determination, computational methods provide a cost-effective alternative to explore the structural and thermodynamic properties of proteins that may be challenging to access through experimentation alone.

To expand our understanding of protein functions and structural organization, we delve into one of the most prevalent post-translational modifications in proteins: the formation of disulfide bonds[1]. These bonds are covalent connections between sulfur atoms in cysteine side chains within a single protein (intramolecular) or between two distinct proteins (intermolecular). Although disulfide bonds were initially regarded as stabilizers of protein structures, it is now clear that their roles and impacts on protein structure and function are more intricate and diverse than previously thought.

Employing computational methods, such as all-atom and coarse-grained molecular dynamics (MD) simulations, offers valuable insights into biomolecule dynamics, conformational changes, and interactions. This talk will focus on demonstrating how the presence or absence of disulfide bonds: (i) affects the mechanical and conformational stability of ribonuclease A from the bovine pancreas (RNase A)[2], (ii) modifies the impact of diverse conditions, such as redox environment, temperature, pressure, salinity, pH, presence of other entities, such as ions and lipid bilayers, on structure and dynamics of various plant non-specific lipid transfer proteins (nsLTPs)[3], and (iii) influences changes in binding patterns between proteins, resulting in differentiation of binding affinities, estimated as binding free energies of HVEM-based peptide inhibitors of the HVEM-LIGHT complex[4].

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Peptide Nucleic Acid Conjugates with Membrane-active Peptides and Their Stapled Analogs as Antimicrobial Agents

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Abstract

Antisense oligonucleotides (ASO) are a rapidly emerging class of therapeutic compounds. One of the most promising nucleic acid mimics, thoroughly investigated in antimicrobial applications, is peptide nucleic acid (PNA). PNA is an artificial nucleic acid mimic with a pseudopeptide, neutral backbone. Its high affinity towards DNA and RNA and sequence specificity provide efficient gene silencing.[1] However, to become an effective antibacterial, PNA has to be internalized into bacteria which is a major challenge, especially in targeting dual-membrane Gram-negatives. A common strategy to improve cellular uptake of PNA is its covalent conjugation to membrane-active peptides that penetrate biological membranes.[2]

Here we present the synthesis and biological evaluation of anti-*acpP* (acyl carrier protein gene) PNA-based hybrids with cyclic membrane-active peptides: $(KFF)_3K$ and anoplin connected to PNA via a non-cleavable ethylene glycol linker or cleavable disulfide bridge. Cyclization of peptides was performed via ring-closing metathesis (RCM) reaction between two alkenyl groups of unnatural amino acids.[3,4]

Antimicrobial activity of obtained peptide-PNA hybrids was determined as minimal inhibitory concentration (MIC) in *E. coli* and *S*. Typhimurium strains. The most promising compounds were examined for their dependence on the bacterial SbmA transporter, as well as their ability to penetrate the bacterial outer membrane. We found that the type of the linker between the counterparts affects the antimicrobial activity of the conjugates. Furthermore, our research shows that cyclic α-helical peptides with stabilized structure exhibit strong bactericidal effects on their own, but poor ability to deliver PNA to Gram-negative bacteria.

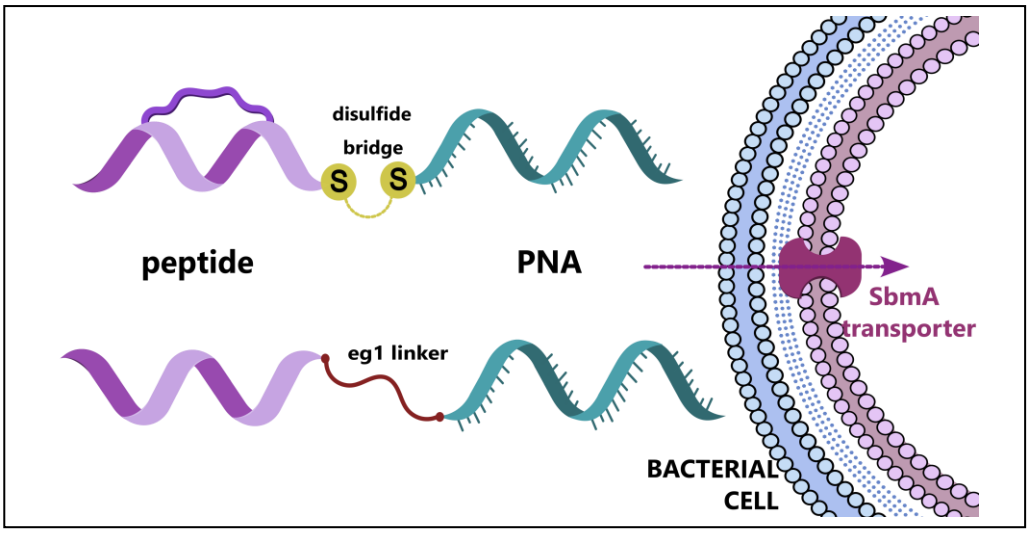

Figure caption: Peptide-PNA conjugates linked via disulfide bridge or ethylene glycol linker as antimicrobial agents.

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Hydrocarbon Stapling to Initiate the Antibacterial Activity of a Cell-penetrating Peptide $(KFF)_3K$

Julia Macyszyn[1], Michał Burmistrz[1], Małgorzata Lobka [1, 2], Joanna Miszkiewicz[1,3], Monika Wojciechowska[1], Joanna Trylska[1]

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Abstract

The high incidence of multidrug-resistant bacteria prompted the search for new antimicrobial agents. We investigated $(KFF)_3K$ - an amphipathic, cell-penetrating peptide (CPP). This peptide can act as a transporter of active molecules through the bacterial membrane without disrupting its continuity. What follows, $(KFF)_3K$ alone shows no antibacterial activity against any studied strain (up to 32 μM) [2].

As a solution to the global problem of antimicrobial resistance, we decided to modify the $(KFF)_3K$ and change its penetrating properties into antimicrobial ones. So far, we found that the stabilization of the secondary structure of peptides correlates with their destructive potential against bacterial membranes and enhancement of their antimicrobial activity [1]. Therefore, we proposed to use the hydrocarbon stapling technique to induce the membrane-active secondary structure of otherwise unstructured $(KFF)_3K$. We introduced non-natural amino acids ((S)-2-(4'-pentenyl)-alanine) at two different positions in the $(KFF)_3K$ sequence. Subsequently, the olefin side chains were cross-linked in the reaction with the Grubbs catalyst to obtain: $(KFF)_3K$[2-6] and $(KFF)_3K$[5-9] [2]. Using circular dichroism spectroscopy, we confirmed that the stapled analogs have a more stable α-helix, especially in a micellar environment. Crucially, both stapled peptides exhibited a considerable increase in antibacterial activity (in the range of 2-16 μM) in comparison to the unmodified peptide. Notably, we showed that stapled analogs inhibited bacterial growth by disrupting their cell wall integrity. In addition, we also verified that hydrocarbon stapling increases the proteolytic stability in chymotrypsin solution. Based on this, $(KFF)_3K$[5-9] showed up to 90% protease resistance. The hemolysis test demonstrated that the stapled analogs had poor hemolytic activity (at the concentration at which they inhibited bacterial growth).

In summary, by using the hydrocarbon stapling technique we induced the antimicrobial activity of one of the CPP - $(KFF)_3K$ [2].

Acknowledgements: This work was supported by National Science Centre Poland (2019/35/D/NZ1/01957)

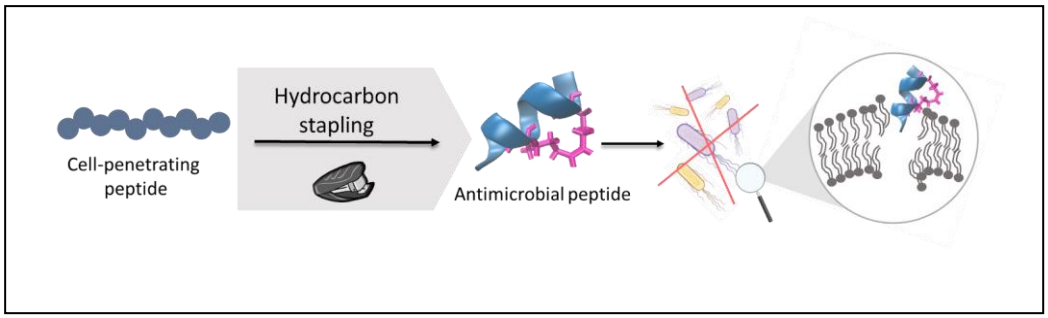

Figure caption: Converting the cell-penetrating peptide into the antimicrobial peptide using the hydrocarbon stapling technique.

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Stapled Anoplins - in Search of a Drug for Pathogens

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Abstract

Combating antibiotic resistance has become one of the biggest challenges facing researchers in the modern world. The overuse of antibiotics to prevent or treat bacterial infections has caused a sharp increase in antibiotic resistance, especially during and after the COVID-19 epidemic [1]. Therefore, it is essential to develop new effective antibacterial drugs against multidrug-resistant bacterial strains.

Antimicrobial peptides (AMPs) are one of the many components of the natural immune systems of living organisms and are increasingly being studied as an alternative to conventional antibiotics [2]. Unfortunately, in some cases AMPs are not stable *in vivo* (e.g., due to proteolytic degradation); they can cause immunological interference or toxicity. AMPs show the ability to specifically bind to their intended targets after adopting the appropriate conformation, often an α-helix. Tuning the specific properties of AMPs by stabilizing their helical conformation makes it possible to refine and reduce their defects.

In this work, an example of stabilizing the active helical structure of one of the AMP representatives - anoplin - will be presented [3]. It was shown that anoplin adopts an active helical structure only in a suitable environment of membrane lipids or lipopolysaccharides [4]. The anoplin helix was stabilized by introducing chemical modifications to its sequence, known as hydrocarbon stapling. The method involves incorporating unnatural amino acids ((S)-2-(4′-pentenyl)-alanine) into the peptide and covalently linking their side chains. The introduction of this modification to anoplin increased its enzymatic stability and improved its antimicrobial activity without showing toxicity to red blood cells [5]. Consequently, very promising derivatives of natural anoplin were obtained showing activity against a wide range of Gram-negative and Gram-positive bacterial strains.

Acknowledgements: This work was supported by National Science Centre Poland (2019/35/D/NZ1/01957)

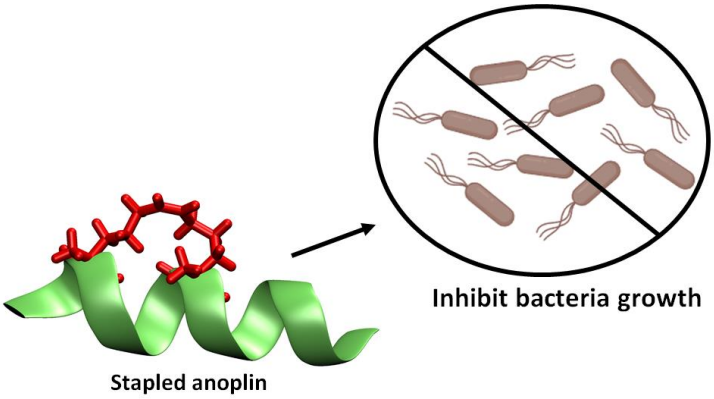

Figure caption: Scheme of the aim of the project.

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Researching the Impact of Korean Popular Culture on Students' Cultural Practices in Ho Chi Minh City

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Abstract

Korean popular culture with waves (Hallyu) have never ended its heat to young people, especially students. Korean popular culture has influenced on the cultural practices of students in the major cities in many countries nowadays. In order to explore the influence of Korean popular culture on students' cultural practices, we apply the approaches of cultural rupture, postmodernism, cultural exchange and contact, and research methods like survey, in-depth interview, comparison. The object of our survey is students in Ho Chi Minh City with more than 600 samples. In Vietnam, Ho Chi Minh City is an educational, cultural, scientific and technological center with a large number of students throughout the country. With 300 years of age, it has been considered a young, dynamic, open, extroverted city, a meeting place for many cultural streams in the world. Research results disclose that some genres of Korean popular culture like costumes, movies, television, music, games, etc. have a certain impact on cultural practices of students in some aspects listed as leisure, consumption, travel preferences, and mindset. However, Korean popular culture is not the strongest or the only one influence and that its role has contributed to enriching and diversifying cultural practices of students, fostering respect for cultural diversity and cultural tolerance. The study also demonstrates that the mass media play an important role in creating a new scenario in the reception and enjoyment of popular culture by students.

Keywords: Popular culture, Korea, cultural practice, Hallyu, Korean cultural wave

Durotaxis and Antidurotaxis Motion onto Gradient Brush Substrates

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Abstract

Using extensive molecular dynamics simulations of a coarse-grained model, we have designed two brush substrates that can cause the motion of fluid droplets by using a gradient in the substrate stiffness. In the first case, the stiffness gradient is controlled through the stiffness of the polymer chains, while in the second case, the stiffness gradient is imposed by varying the grafting density of the polymer chains. In the first case, durotaxis motion is observed, while in the second antidurotaxis motion, that is droplet motion from stiffer toward softer parts of the brush substrate. A full investigation of the relevant parameters (*e.g.* viscosity, droplet size, *etc.*) is conducted and the underlying mechanisms of the droplet motion for each case are explored. Thus, our findings indicate further possibilities in the area of nanoscale motion without external energy supply.

Figure caption: Durotaxis and antidurotaxis motion onto gradient brush substrates

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New Study on the Age of Tertiary Sediments in the Na Duong Basin (Northern Vietnam) Based on Palynological Analysis

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Abstract

Na Duong, the largest brown coal pit in Vietnam, plays a pivotal role in the economic landscape. Located within the Na Duong Basin (Fig. 1A), is characterized by two distinct units: the lower Na Duong Formation (Fig. 1B) and the upper Rinh Chua Formation (Fig. 1B). These formations were deposited along the Cao Bang-Tien Yen Fault (Fig. 1A) in northern Vietnam, which exhibits a subparallel alignment with the Red River Fault Zone (Fig. 1A), a region of considerable geotectonic significance.

The precise age of the Na Duong Basin has been a subject of ongoing discussion. Previous concepts have proposed either a Miocene-Pliocene or Oligocene age for the infill of this basin. However, recent studies, as detailed in Wysocka et al. (2020), propose a late Oligocene, Oligocene-Eocene, and/or Eocene age for this deposit.

Palynological analyses were carried out on seventeen samples from the Na Duong Formation and six samples from the Rinh Chua Formation. Six samples from the Na Duong Formation, as well as all samples from the Rinh Chua Formation, possessed a sufficient quantity of palynomorphs to conduct palynological analysis. A total of 44 sporomorph taxa were identified, comprising 9 taxa of plant spores, 7 taxa of gymnosperm pollen, and 28 taxa of angiosperm pollen. Both formations exhibited similar pollen assemblages, with predominant angiosperm and gymnosperm pollen and low taxonomical diversity. The angiosperm component is dominated by *Caryapollenites* (*Carya*), *Periporopollenites* (*Liquidambar*), *Tricolporopollenites indeterminatus*, and *Ulmipollenites*. The primary distinction between the assemblages of the Na Duong and Rinh Chua Formations lies in the elevated occurrence of *Persicarioipollis* and the presence of *Chenopodipollis* and *Graminidites* (indicative of herbaceous plants) within the latter. Most of the recognized taxa indicate a warm-temperate climate. Nevertheless, certain pteridophytes and representatives of the Cornaceae, Loranthaceae, and Dipterocarpaceae families are associated with subtropical and tropical environmental conditions.

Basing on comparison with palynofloras from the vicinity, the composition of the assemblages corresponds well with the pollen assemblages of the the Maoming and Nanning Basins from Southern China. In the Maoming Basin, the pollen assemblages examined in the Na Duong Basin exhibit the closest resemblance to a lowermost Oligocene PC1 pollen assemblage from the Shangcun Formation (as detailed in Wysocka et al. (2020)). This assemblage is characterized by the frequent presence of

gymnosperm pollen, significant spore abundances, and an abundance of angiosperm pollen representing temperate taxa such as Hammamelidaceae, *Liquidambar*, *Carya*, and *Quercus*. The presence of *Tsuga* and *Persicaria* pollen (as detailed in Wysocka et al. (2020)) supports the argument for an Oligocene age. Sediments in the Nanning Basin are also considered to be an Oligocene age. Consequently, an Early Oligocene age is proposed for both the Na Duong and Rinh Chua Formations. The lack of significant differences in the taxonomic compositions of both formations under study suggests that the Rinh Chua Formation was deposited in close temporal proximity to the Na Duong Formation. Furthermore, both of these assemblages bear a striking resemblance to previously studied palynological spectra from the Cao Bang Basin (see Fig. 1A) (Wysocka et al., 2018).

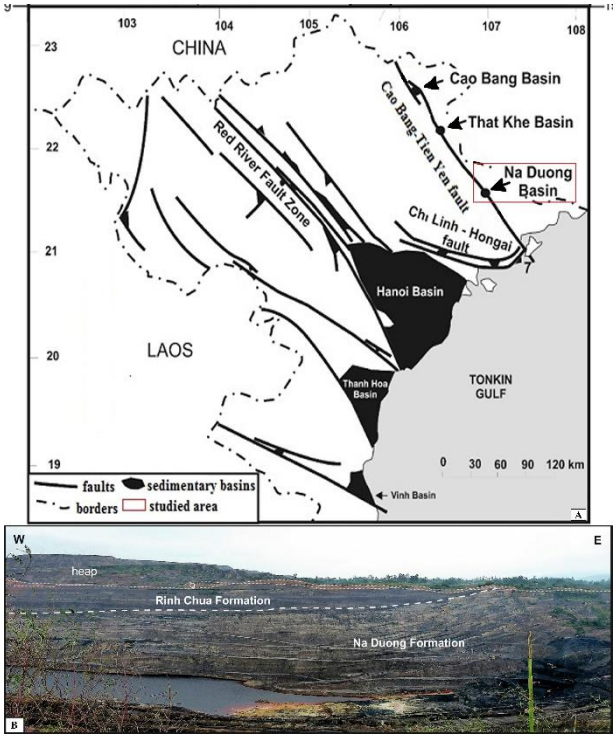

Figure caption: Location of the study area (modified after Wysocka et al. 2020). (A) Position of the Na Duong Basin; (B) An overview of the Na Duong coal mine with the boundary between the Na Duong and Rinh Chua Formations indicated by a dashed line.

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Fixed Points of Monotone Operators Via Measure of Noncompactness

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Abstract

Fixed point theory is very useful in studying solutions of integral and differential equations. A promising technique in this theory involves measures of noncompactness. Darbo [1] was the first to use the Kuratowski measure of noncompactness α, and proved that if T is a continuous self-mapping of a nonempty bounded closed and convex subset C of a Banach space E such that

$$\alpha\big(T(\Omega)\big) \leq k\alpha(\Omega)$$

for all $\Omega \subset C$, where $k < 1$, then T has a fixed point in C. Darbo's theorem is a generalization of Schauder's fixed point theorem and includes the existential part of Banach's fixed point theorem. Next, the Hausdorff measure of noncompactness was used by Gohberg, Goldenštein and Markus in [2]. After that, Sadovskiĭ [3] generalized the Darbo's result for any measure of noncompactness. In 1968, Szufla [4] applied the Darbo's theorem to solve the initial-value problem in Banach spaces. Recently, several papers have appeared that apply the concept of measures of noncompactness in the study of the existence and behavior of solutions of different kinds of functional equations (see [5-8]). The common characteristic in applying the fixed point existence theorems is to find a bounded closed and convex subset in a given Banach space, which is transformed into itself by a continuous operator.

In this paper we show the counterparts of Darbo– Sadovskiĭ's theorem for a monotone, not necessarily continuous, mapping $T : X \to X$ under the assumption

$$\mu(T(\Omega)) < \mu(\Omega)$$

for any bounded subset Ω in an ordered complete metric space X, where μ is a measure of noncompactness on X. As applications, we prove the existence of solutions for some functional-integral equations and ordinary differential equations. The choice of a suitable measure of noncompactness plays a key role in solving the equations. Several examples are provided to illustrate our results.

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Empirical Validation of Graph Structure Learning for Citation Network Applications

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Abstract

This work investigates the classification accuracy of Graph Structure Learning methods in the domain of Graph Neural Network (GNNs), specifically focusing on paper classification within citation network datasets. While GNNs excel at processing non-Euclidean structured data, a major drawback is their assumption of a fixed, known underlying graph, which often doesn't hold in real-world scenarios.

In this work, we aim to:

- Review state-of-the-art graph structure learning (GSL) methods.
- Empirically validate GSL methods using citation network datasets.
- Analyze the mechanisms of these approaches and the influence of hyperparameters on model behavior.

Our key finding highlights the superiority of graph-based neural networks over traditional neural networks, such as Multilayer Perceptrons, for graph-based datasets. We showcase an evolutionary progression of Graph Structure Learning techniques, starting with Graph Convolutional Networks (GCN), advancing to Graph Attention Networks (GAT), and finalizing in Discrete DGM (dDGM). This progression represents a paradigm shift in graph data handling, ultimately leading to enhanced performance, as confirmed by validated results.

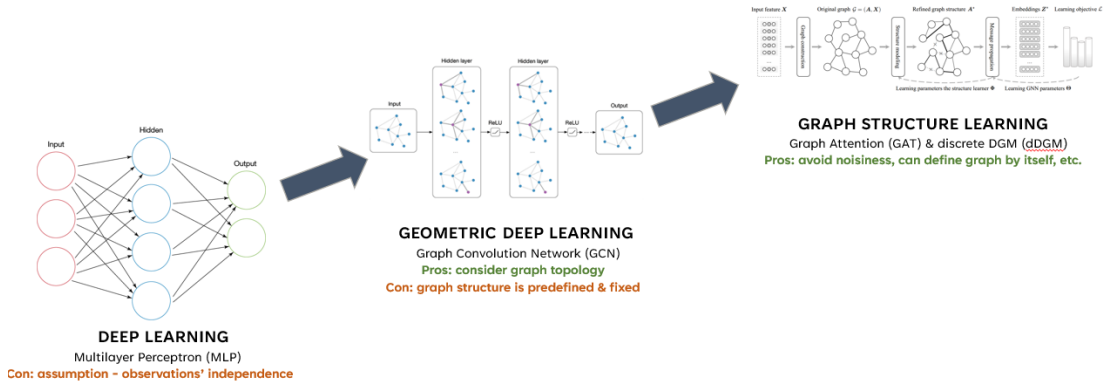

Figure caption: Paradigm shift of Graph Structure Learning techniques.

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The Internet of Bridge Things: A Reviewing of AI-assisted Structural Health Diagnostic

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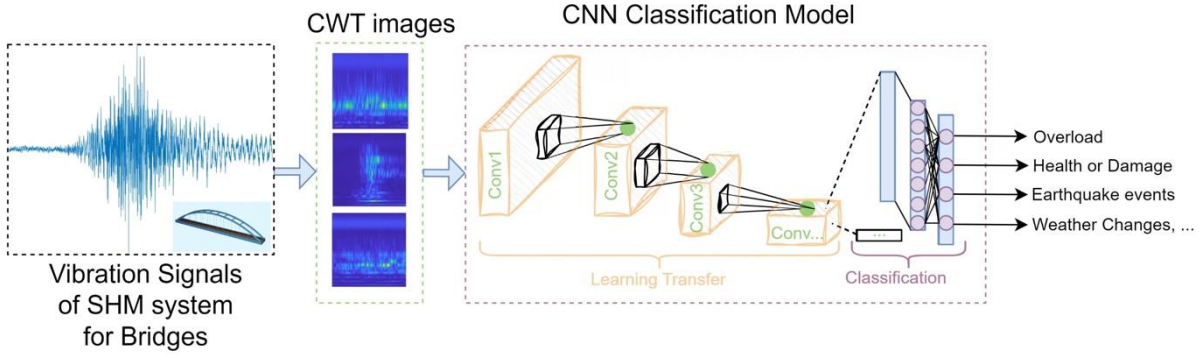
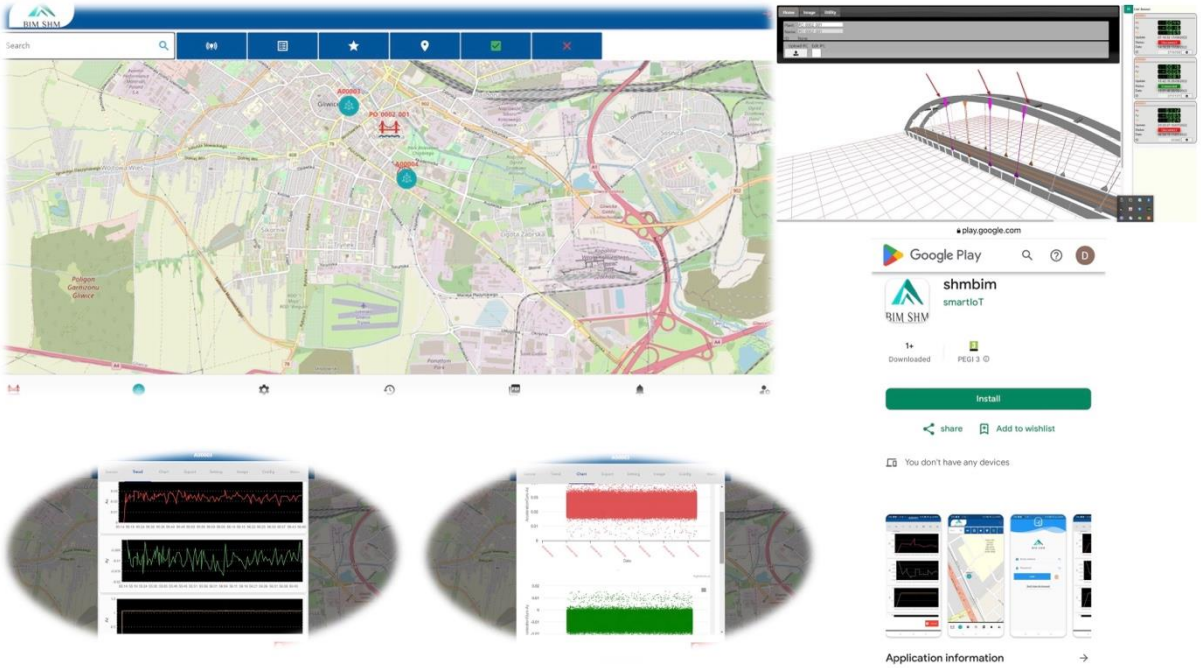
Abstract

The study presents a review of the internet of bridge health things using CWT-engaged CNN approaches for vibration-based structural health monitoring (SHM) of the existing bridge structures under various events. The SHM system is a valuable tool for tracking the potential structural problems such as: overload, cracks, failures, earthquake events, and weather changes. To enhance the signal processing and management of SHM system for bridges more efficiently and reliably, we can consider integrating the robust CWT images of vibration signals into CNN classification and Regression models for predicting structural issues. The CWT algorithm transforms time-domain vibration signals into the time-frequency spectrogram images, as input in CNN models. The proposed approach is useful tool of emerging technique for monitoring health conditions of bridges, as well as other structures (buildings, tunnels, and dams) in real-time.

CWT-engaged CNN Classification or Regression Models



Vibration-based Structural Health Monitoring System using The Internet of Things



DFT Study of Structural and Electronic Properties of Double Perovskites Ba_2MnWO_6 and Ba_2TiMnO_6

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Abstract

In recent years, double perovskites with the chemical formula $A_2BB'O_6$ (A = alkaline earth or rare-earth metal; B, B' = transition metals) oxides have attracted significant attention due to their prospective applications as magnetocaloric [1] and optoelectronic materials [2]. In this report, we present the results of Density Functional Theory (DFT) calculations for two magnetically ordered double perovskites with semiconducting characteristics, i.e. Ba_2MnWO_6 and Ba_2TiMnO_6.

Our calculations employed the Gennerlized Gradient Approximation (GGA) and on-site Coulomb interaction of localized 3*d* electron (Hubbard *U* parameter) (GGA+*U*) to investigate the magnetic and electronic properties of these compounds. We studied several magnetic configurations, including both nonmagnetic, ferromagnetic and antiferromagnetic. In the ordered state, we assume that Mn^{2+} moments are arranged in either the (001) or (111) planes. According to our findings, the most stable magnetic structure is antiferromagnetic, with collinear Mn spins aligned along the [001] direction and an ordered moment μ_{ord} of roughly 4.42 μ_B and 2.56 μ_B for Ba_2MnWO_6 and Ba_2TiMnO_6, respectively. The careful analysis of the density of states (DOS) and the electronic band structure (EBS) reveals that Ba_2MnWO_6 is an indirect narrow band gap semiconductor with semiconducting energy gap of approximately E_g = 0.36 eV [3], whereas Ba_2TiMnO_6 is a direct band gap semiconductor with an energy gap E_g of 0.98 eV [4]. Furthermore, the effects of *U-J* parameters were examined for the semiconducting energy gap E_g. We found that in constrast to μ_{ord}, E_g shows a noticeable upward trend with *U*, reaching a value of 1.76 eV and 1.27 eV at *U* = 4 eV, *J* = 1 eV for Ba_2MnWO_6 and Ba_2TiMnO_6, respectively.

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Kink-Meson Inelastic Scattering

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Abstract

The subject of this talk is the quantum theory of inelastic scattering of a meson with a kink. In this talk, we first review the linearized soliton perturbation theory developed in recent years, which is particularly simple in the one-kink sector. Using it, the amplitude and probability of kink-meson inelastic scattering can be simplified into a perturbative problem in the kink frame. Then we consider the inelastic scattering of a meson off of a kink in a (1+1)-dimensional scalar quantum field theory. At leading order there are three inelastic scattering processes: (1) meson multiplication (the final state is two mesons and a kink); (2) Stokes scattering (the final state is a meson and an excited kink); (3) anti-Stokes scattering (the initial kink is excited and the final kink is de-excited). For the first time, we calculate the leading-order probabilities of these three processes and the differential probabilities for final-state mesons with different momenta. We first obtain general results for arbitrary scalar kinks and then apply them to the kinks of the ϕ^4 double well model to obtain analytical and numerical results. Finally, we believe that our method can be generalized to higher dimensions, such as the case of monopoles.

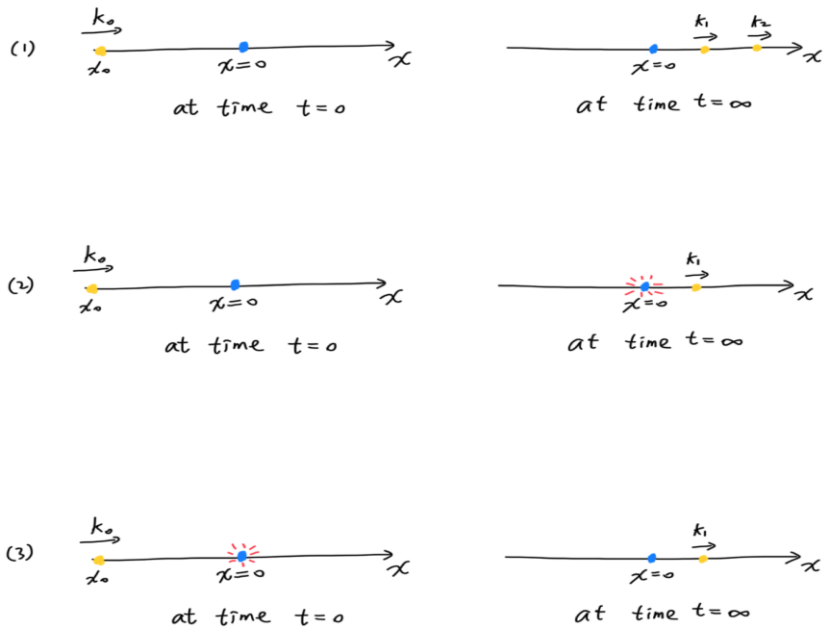

Figure caption: Three expected processes of kink-meson inelastic scattering. The yellow dots represent mesons, and the blue dots represent kinks. At the initial time $t=0$, the mesons are located at $x=x_0$ and have a momentum of k_0, while the kinks are located at $x=0$ (since we are discussing in the center-of-mass frame and the kink mass is much larger than the meson mass, we can assume that the kink position remains at $x=0$ before and after scattering). The three processes are: (1) before and after scattering, the kink is in the ground state, and one meson splits into two, which we call meson multiplication; (2) the number of meson remains unchanged before and after scattering, and the kink is excited from the ground state to the excited state, which we call Stokes scattering; (3) the number of meson remains unchanged before and after scattering, and the kink is de-excited from the excited state to the ground state, which we call anti-Stokes scattering.

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Effect of A-site Cation Substitution in A_2MgWO_6 Double Perovskites Doped with Dy^{3+} (A = Ca, Sr, Ba) on the Crystal Structure, Luminescence and Temperature Sensing Performance

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Abstract

Structure change resulting from cation substitution has been demonstrated as an effective way to tune the temperature sensing performance[1]. This study presents the impact of cation substitution on the optical properties and temperature sensing performance of A_2MgWO_6 (A = Ca, Sr, Ba) doped with 2%Dy^{3+}, 2%Li^{+}. All samples were successfuly synthesized by using the co-precipitation method[2,3]. Replacing larger Ba^{2+} ions with Ca^{2+} and Sr^{2+} ions resulted in structural changes from cubic to monoclinic and tetragonal, respectively. These structural modifications influenced the crystallographic symmetry site of Dy^{3+}in the lattice, shifting the emitted light color from whitish to yellowish and causing a blue-shift of the charge transfer band (CTB). Additionally, the lifetime of the $^4F_{9/2} \rightarrow 6H_{13/2, 15/2}$ transitions decreased significantly from 749 μs for Ba to 199 μs for Sr and 146 μs for Ca due to the reduced local symmetry of Dy^{3+}. Furthermore, the fluorescence intensity ratio technique was employed to evaluate the thermal sensing properties of 2%Dy^{3+}-doped samples between 80 and 325 K. Under 266 nm excitation, the maximum relative sensitivity of the samples increased notably from 2.26%/K for Ba to 3.04%/K for Ca and 4.38%/K for Sr sample. These findings provide insights into the effects of compositional changes on optical properties and offer a promising approach for tailoring temperature sensing performance.

Acknowledgment

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Molecular Dynamics Simulation of the Coalescence of Droplets

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Abstract

Droplet coalescence is commonly encountered in nature and is also relevant in various technologies, such as microfluidics. I will present our results on the coalescence of surfactant-laden water droplets, which have been obtained by means of a coarse-grained (CG) force field. In particular, I will discuss the details of the coalescence mechanism and the dynamics of bridge growth.

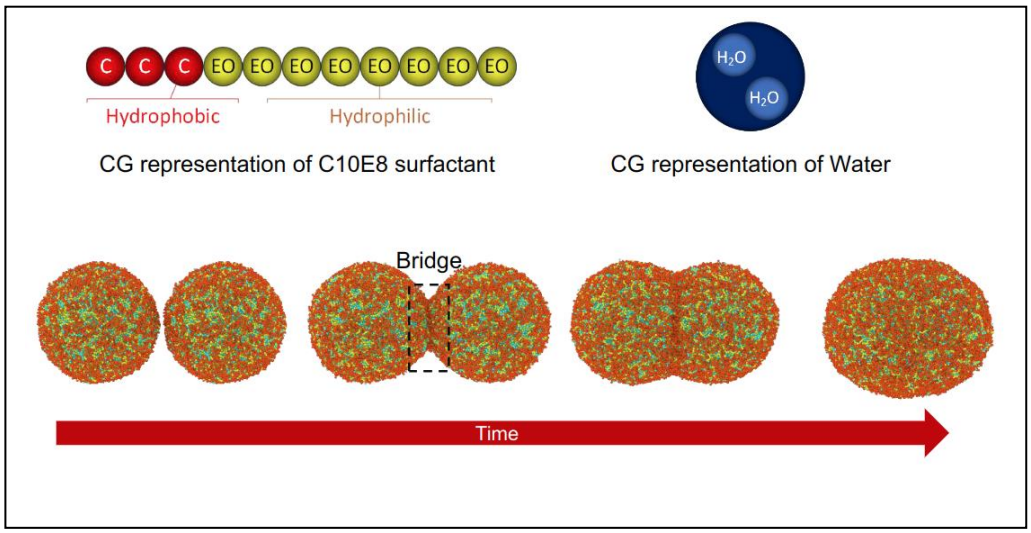

Figure caption: Coalescence of surfactant-laden droplets.

Impact of Metallicity on Far-infrared Line Cooling in the Embedded Cluster Gy 3–7 in the Outer Galaxy

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Abstract

Star formation is ubiquitous in the Galaxy, but the physical and chemical conditions in star-forming sites might differ due to the environment. For example, due to the negative metallicity gradient, abundances of molecules and dust are expected to decrease with the distance from the Galactic Center, and subsequently influence the cooling budget and efficiency of star formation. In this talk, I will present the study aiming to investigate the role of metallicity on far-infrared line cooling in the embedded cluster Gy 3-7 in the Outer Galaxy, which has a metallicity (Z) of 0.55-0.73 Z_sun using the SOFIA/FIFI-LS observations. I will discuss the possible effect of metallicity, as well as the physical conditions and ultraviolet radiation field strengths in the cluster.

Strategic Enhancement of Vietnam's Red River Delta Primary School Libraries

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Abstract

This research critically examines the primary school library system in Vietnam's Red River Delta using a transdisciplinary methodology. Integrating insights from library science, education, marketing, and psychology, the study employs a mixed-methods approach, including a literature review, surveys with educators and librarians, and interviews with school principals across the diverse schools in 10 provinces of this region. The findings reveal key operational challenges and stakeholder perceptions, leading to the development of a strategic model for library improvement. This model, informed by a comprehensive SWOT analysis, offers practical recommendations for national application, aiming to advance the region's educational library systems and contribute to global librarianship discourse.

Keywords: primary school library, operation, organization, Red River Delta, Vietnam

The Interdependence of Happiness and Filial Piety Within the Family – A Study in Vietnam

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Abstract

Filial piety is one of the most important values in Vietnam, as it is in a number of East Asian countries, it is an expression of children's respect, gratitude, and care for their parents. While filial piety may bring joy to parents and is a personal duty for offspring, it can also be a pressure for children. Hence, in recent years, some studies considered filial piety as two dimensions instead of one dimension.

This study focused on clarifying the relationship between filial piety and perceived family happiness with 385 adult offspring who lived in Vietnam at the time of study. The Dual Filial Piety Scale (DFPS) and the Interdependent Happiness Scale (IHS) were used.

The results showed that participants regularly engaged in aspects of filial piety and there was no contradiction between authoritarian filial piety (AFP) and reciprocal filial piety (RFP). Filial piety can predict family happiness at a fairly high level.

This result, besides showing the importance and value to the family, also gives a multi-dimensional and comprehensive view of filial piety. At the social level, upholding the value of filial piety is both the basis for building family happiness, as well as making an important contribution to the implementation of social security in the family.

Keywords: Filial piety, dual filial piety, happiness, family happiness, filial piety and family happiness.

Factors Affecting Digital Transformation in Tourism Human Resource Training: Case Study of Central Coastal Provinces

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Abstract

The main purpose of this study is to find factors influencing digital transformation in training tourism business human resources within the Central provinces of Vietnam. Accordingly, the study synthesizes many opinions of experts in the tourism industry from 221 hotels and opinions of former tourism majors from schools with tourism training in the central coastal provinces for a long time from Thanh Hoa to Binh Thuan on the factors that determine the quality of tourism human resource training. The study used R software to analyze data. Research results show that there are 6 digital transformation factors in tourism human resource training in the Central Coast provinces including: Cost; Human resources (HR); Information technology (IT) infrastructure; Support from the government; Macro policy; and digitalization trends in tourism. Research results help policymakers make informed decisions as well as provide timely support for the digital transformation process in training quality human resources capable of adapting to today's new conditions.

Keywords: Training quality, tourism human resources, central coast.

POSTERS

P01: Unprotected Edge Modes in Quantum Spin Hall Insulator Candidate Materials

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Abstract

The experiments in quantum spin Hall insulator candidate materials, such as HgTe/CdTe and InAs/GaSb heterostructures, indicate that in addition to the topologically protected helical edge modes, these multilayer heterostructures may also support additional edge states, which can contribute to scattering and transport. We use first-principles calculations to derive an effective tight-binding model for HgTe/CdTe, HgS/CdTe, and InAs/GaSb heterostructures, and we show that all these materials support additional edge states which are sensitive to edge termination. We trace the microscopic origin of these states back to a minimal model supporting flat bands with a nontrivial quantum geometry that gives rise to polarization charges at the edges. We show that the polarization charges transform into additional edge states when the flat bands are coupled to each other and to the other states to form the Hamiltonian describing the full heterostructure. Interestingly, in HgTe/CdTe quantum wells the additional edge states are far away from the Fermi level so that they do not contribute to the transport, but in the HgS/CdTe and InAs/GaSb heterostructures they appear within the bulk energy gap, giving rise to the possibility of multimode edge transport. Finally, we demonstrate that because these additional edge modes are nontopological it is possible to remove them from the bulk energy gap by modifying the edge potential, for example, with the help of a side gate or chemical doping.

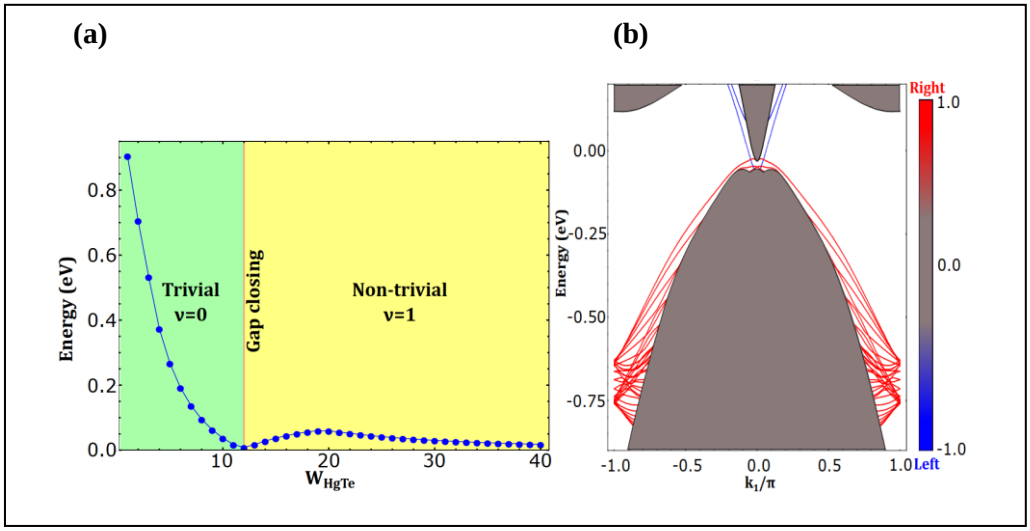

Figure caption: Energy gap E_{gap} and topological invariant ν as a function of the quantum well thickness W_{HgTe} in a $CdTe_{10}/HgTe_{W_{HgTe}}/CdTe_{10}$ heterostructure. (b) Edge state spectrum of a topologically nontrivial $CdTe_{10}/HgTe_{16}/CdTe_{10}$.

P02: **Competitive Destination Analysis in Southeast Asia**

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Abstract

Asia-Pacific has risen to prominence in recent years as the fastest-growing tourism and travel region, challenging the traditional dominance of Europe and North America (Henderson, 2015). While the focus is frequently on Eastern, South East Asia is also seeing substantial growth and a reshaping of demand and supply. Southeast Asian countries view tourism as a means to generate income and employment (Trupp & Dolezal, 2020). Many visitors are attracted to the region's combination of rich natural resources and price competitiveness, with the latter being its greatest advantage relative to other countries in the broader Asia-Pacific region. In addition, the region's above-average air transport infrastructure continues to improve at a rapid pace, especially in regard to the number of operating airlines and route capacity. In 2019, Southeast Asia receiving 143.1 million international tourists, with the countries hosting the largest number of international visitors being Thailand (39.8 million international tourists), Malaysia (26.1 million international tourists), and Singapore (19.1 million international tourists) (Trupp et al., 2020). Howerver, this region's greatest weakness is environmental sustainability, which has been impacted by deforestation, an increasing number of threatened species and insufficient wastewater treatment (The World Economic Forum, 2019).

Table 1. International tourist arrivals to Southeast Asian countries (Unit: Million Visitors)

Countries	2015	2016	2017	2018	2019
Thailand	29.9	32.6	35.5	38.2	39.8
Malaysia	25.7	26.8	25.9	25.8	26.1
Singapore	15.2	16.4	17.4	18.5	19.1
Vietnam	7.9	10.0	12.9	15.6	18.0
Indonesia	10.4	12.0	14.0	15.8	16.1
Philippines	5.4	6.0	6.5	7.2	8.2
Cambodia	4.8	5.0	5.6	6.2	6.7
Myanmar	4.7	2.9	1.4	1.4	4.3
Laos	4.7	4.2	3.9	4.2	4.6
Brunei	0.2	0.2	0.3	0.3	0.2

Source: VNAT, 2020

Competition in the tourism industry in the Southeast Asia region has become a crucial factor as countries within the region strive to attract tourists and develop revenue sources. According to the World Economic Forum (2019) report, the Philippines had the fastest rate of improvement, moving up four places to rank 75th globally. Though relatively isolated from air connections for many years, has seen tourism growth as access options have improved (Trupp et al., 2020). The country showed impressive improvement on overall infrastructure (90th to 80th) and information & communication technologies (ICT) readiness (86th to 82nd), but still faces challenges when it comes to safety and security (135th). On the other hand, Singapore had the greatest percentage decline in score (losing four places) but remains the subregion's most competitive tourism country, ranking 17th globally. It has a world-class business environment (2nd), human resources and labour market (5th), ICT readiness (15th), safety and security (6th), Tourism policy and conditions (2nd) and overall infrastructure (3rd). Despite this, Singapore dropped from first to third for international openness, due to increased visa requirements (16th to 50th) and a drop in scores for its natural (103rd to 120th) and cultural resources (28th to 38th). Cambodia (98th) remains the lowest scorer in South-East Asia, trailing the subregion on the Enabling Environment (106th) and Infrastructure (101st) subindexes. Thailand (31st) has SouthEast Asia's largest tourism and travel GDP, which is reinforced by some attractive natural resources (10th) and most efficient tourist services infrastructure (14th).

In 2019, Vietnam welcomed over 18 million international visitors, surpassing Indonesia's 16.1 million. The growth in international arrivals to Vietnam, with a remarkable increase of 16.2%, significantly outpaced other countries in the region, such as Thailand (4.2%), Indonesia (1.9%), and Singapore (3.2%) (VNAT, 2019). Vietnam's tourism competitiveness has improved significantly, rising from the 75th position out of 141 economies in 2015 to 67th out of 136 in 2017 and further improving to 63rd out of 140 in 2019 (The World Economic Forum, 2019). In 2019, Vietnam excelled in several key competitiveness indicators, with the highest rankings in the following categories: Price Competitiveness (22nd); Cultural Resources (29th); and Natural Resources (35th). In the Southeast Asian region, Vietnam's Cultural Resources ranked second, trailing behind Indonesia, and its Natural Resources ranked third, after Thailand and Indonesia. These rankings highlight Vietnam's significant comparative advantages in terms of cultural and natural resources within the region and on a global scale. Vietnam has a favorable geographical location including a long coastline with many beautiful landscapes and beaches, islands and archipelagos (Cooper, 2000; London, 2020; Nguyen Van et al., 2022; Truong Van, 2014). Besides, the climate is tropical - this is a huge strength for Vietnam's tourism industry.

Table 2. Ranking tourism and travel competitiveness in Southeast Asia

	(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)	(9)	(10)	(11)
Singapore	6.0	6.4	5.6	5.6	6.1	6.1	4.8	5.0	4.3	2.2	2.5
Malaysia	5.5	5.9	5.3	5.4	5.4	4.8	4.5	6.3	4.0	3.8	2.6
Thailand	4.9	4.8	5.0	5.1	5.2	5.2	3.9	5.8	3.6	4.8	2.6
Indonesia	4.7	5.4	4.5	4.9	4.7	5.9	4.3	6.2	3.5	4.5	3.2
Vietnam	**4.4**	**5.6**	**5.0**	**4.8**	**4.3**	**4.1**	**3.7**	**5.9**	**3.8**	**3.8**	**2.9**
Brunei	4.8	6.1	5.5	4.6	5.4	3.4	3.7	6.6	4.1	2.4	1.1
Philippines	4.3	3.6	4.8	5.0	4.4	4.9	3.5	5.9	4.0	3.8	1.8
Laos	4.4	5.3	4.5	4.6	3.4	4.8	3.0	5.9	3.7	2.9	1.3
Cambodia	3.8	5.1	4.0	4.2	3.9	5.0	3.5	5.6	3.4	3.0	1.6

(1) Business Environt ment, (2) Safety & Security, (3) Health & Hygiene, (4) Human Resources & Labor Market, (5) ICT Readiness, (6) Prioritization of Travel & Tourism, (7) International Openness, (8) Price Competitiveness, (9) Environmental Sustainability, (10) Natural Resources, (11) Cultural Resources and Business Travel.

Source: The World Economic Forum, 2019

However, Vietnam ranks lower than other countries in Southeast Asia in several key indices, including Environmental Sustainability, Tourism Service Infrastructure, and Tourism Sector Prioritization; especially the ranking visa requirements index (The World Economic Forum, 2019). Vietnam has just exempted visas for citizens of 22 countries, compared to Thailand at 61, Malaysia at 155, Singapore at 158, Indonesia at 169.

In conclusion, despite South-East Asia ’s many strengths, the region does face several challenges. Although tourist service infrastructure has become more developed, most South-East Asia countries still have more region’s greatest competitiveness constraint. Many countries suffer from high air pollution, water stress, below-average levels of wastewater treatment, endangered wildlife and forest loss. In order to maintain and increase its market share in the tourism sector, Vietnam needs to uphold and enhance the quality of tourism services, conserve and develop tourism resources sustainably, and continually explore new opportunities within the tourism industry.

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P03: **Objectivity in the Oscillator-spin Model**

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Abstract

We investigate the objectivity in a simple harmonic oscillator interacting with the large collections of 1/2-spin environments, which is expressed by the Spectrum Broadcast Structure (SBS). We calculate two measures for SBS, decoherence factor and a generalized overlap, which characterize the SBS structure. Assumption that a harmonic oscillator influences spins mainly as a classical state with little back reaction from spins (Born-Oppenheimer approximation) leads to an effective Hamiltonian for spins by replacing a position operator of a harmonic oscillator with its time-dependent classical trajectory. The periodic effective Hamiltonian allows us to use the Floquet theory and the high frequency expansion is utilized.

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P04: The Coexistence Region in the Van der Waals Fluid and the Liquid-liquid Phase Transitions

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Abstract

Cellular membraneless organelles are thought to be droplets formed within the two-phase region corresponding to proteinaceous systems endowed with the liquid-liquid transition. However, their metastability requires an additional constraint—they arise in a certain region of density and temperature between the spinodal and binodal lines. Here, we consider the well-studied van der Waals fluid as a test model to work out criteria to determine the location of the spinodal line for situations in which the equation of state is not known. Our molecular dynamics studies indicate that this task can be accomplished by considering the specific heat, the surface tension and characteristics of the molecular clusters, such as the number of component chains and radius of gyration.

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P05: The Driving Force for Co-translational Protein Folding is Weaker In the Ribosome Vestibule due to Greater Water Ordering

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Abstract

Interactions between the ribosome and nascent chain can destabilize folded domains in the ribosome exit tunnel's vestibule, the last 3 nm of the exit tunnel where tertiary folding can occur. Here, we test if a contribution to this destabilization is a weakening of hydrophobic association, the driving force for protein folding. Using all-atom molecular dynamics simulations, we calculate the potential-of-mean force between two methane molecules along the center line of the ribosome exit tunnel and in bulk solution. Associated methanes, we find, are half as stable in the ribosome's vestibule as compared to bulk solution, demonstrating that the hydrophobic effect is weakened by the presence of the ribosome. This decreased stability arises from a decrease in the amount of water entropy gained upon the association of the methanes. And this decreased entropy gain originates from water molecules being more ordered in the vestibule as compared to bulk solution. Therefore, the hydrophobic effect is weaker in the vestibule because waters released from the first solvation shell of methanes upon association do not gain as much entropy in the vestibule as they do upon release in bulk solution. These findings mean that nascent proteins pass through a ribosome vestibule environment that can destabilize folded structures, which has the potential to influence co-translational protein folding pathways, energetics, and kinetics.

P06: Aggregation Rate of Amyloid Beta Peptides is Controlled by Beta-Content in Monomeric State and Mechanical Stability of Fibrillar Structure

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Abstract

The formation of the fibrillar structure and oligomers of amyloid proteins/peptides is believed to be associated with neurodegenerative diseases such as Alzheimer's disease, Parkinson's disease, amyotrophic lateral sclerosis, etc. Since the rate of aggregation can influence neurotoxicity, the search for key factors controlling this rate is of paramount importance. Recently, evidence has been found that the rate of protein aggregation is related to the mechanical stability of the fibrillar structure and the content of beta in the monomeric state in such a way that the higher the mechanical stability or the beta content, the faster the formation of fibrils. However, this conclusion was supported by limited data.

In this report, we extend the previous study to a larger dataset, including the wild type of Aβ42 peptide and its 20 mutants, whose aggregation rate was measured experimentally. Using all-atom steered molecular dynamics (SMD) and conventional molecular dynamics (CMD) simulations, we can access the mechanical stability of the fibril structure and the beta content in the monomeric state. Our result supports the hypothesis that mechanical stability and beta content are related to the aggregation rate. Since estimation of the aggregation rate using all-atom simulations is nearly forbidden by current computational capabilities, our result is useful for predicting it based on information obtained from CMD for monomers and SMD simulations for fibrils, which are computationally feasible.

P07: Coarse-grained Molecular Dynamics of Intrinsically Disordered Proteins

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Abstract

We employ molecular dynamics (MD) and coarse-grained (CG) methods to study intrinsically disordered proteins and their assemblies. Firstly, we use the CG pseudo-improper-dihedral model that we have developed recently [1,2] to study α-synuclein in a broad range of concentrations and temperatures. Our simulation results show that α-synuclein assembles into network structures that percolate at sufficient protein concentrations. We discuss the role of particular contacts in the α-synuclein networks, and show that the majority of them are based on electrostatic interactions between the N- and C-termini. We also investigate how the density of α-synuclein clusters depends on protein concentration and temperature. Secondly, we employ the Martini 3 model [3] to characterize conformations of galectin-3, which is mixed-folded protein comprising an intrinsically disordered N-terminal tail and a carbohydrate recognition domain. We follow the methodology of Thomasen et al. [4] to rescale protein-water interactions, and obtain a conformational ensemble fully consistent with data from small angle X-ray scattering experiments [5]. Our simulation results show that galectin-3 exhibits large-scale fluctuations between compact and extended conformations.

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P08: Hydrogenation of Two-dimensional Material Germanene Using MD and DFT Simulation Methods

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Abstract

The electronic properties of the 2D hexagonal $P6_3mc$ space group germanene are investigated using the density function theory method. The band structures and vibration properties of germanene, full hydrogenated germanene (FGeH), semi-hydrogenated germanene on top high buckling ($SGeT_1$), semi-hydrogenated germanene on top low buckling ($SGeT_2$) are analyzed. It was shown that the band structure of three models transits germanene from semimetal to metal and again back to semimetal, prooving that the less hydrogen adsorbed on germanene, the more likely it is metal. The phonon dispersion showed that germanene and full hydrogenated germanene (FGeH) were more stable than the other two models

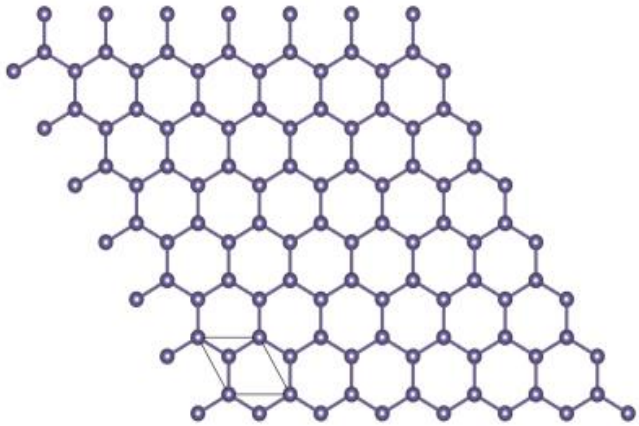

Figure caption: 2D honeycomb germanene model with hydrogen atoms on the surface.

Keywords: density functional theory, two-dimensional, germanene, hydrogenation.

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P09: **Vietnam: The Next Asian Tiger?**

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Abstract

Vietnam is on its way to becoming a significant economic development success story. This Southeast Asian country has been recognized as one of the best performing economies in the world over the past few decades.

The spectacular growth of large emerging economies in East Asia over the past six decades has amazed economists, businesses, and governments. First, it was Japan in the post-World War II era [1], followed by the Four Tigers (Hong Kong, Singapore, South Korea, and Taiwan) in the 1960s [2], and then China's growth miracle since 1978 [3]. Vietnam is seen by many experts as the next emerging giant. For instance, in 2005, Vietnam was included in Goldman Sachs' Next Eleven. This was a group of eleven countries whom they believed had the greatest potential to become the next group of major economies in the 21st century, based on a set of indicators, such as education and demographics [4]. In 2009, the Economist Intelligence Unit included Vietnam in CIVETS [5]. This was a group of six countries whom they touted to become the next generation of emerging market economies, based on factors such as low public debt, favorable demographics and rising levels of foreign direct investment (FDI). PricewaterhouseCoopers (PWC) predicted that Vietnam could be one of the fastest growing economies in the world over the 2015–2050 period [6].

Current signs show that Vietnam is well on its way to imitating the growth miracles of Japan, the Four Tigers, and China. The average annual growth rate of Vietnam's GDP and GDP per capital in the last three decades reached 6-7% per year. Even during the COVID-19 pandemic, Vietnam is still one of only a few economies in the world to achieve GDP growth in 2020. GDP growth slowed down to 2.58% in 2021 due to the appearance of the Delta variant but rebounded to more than 8% in 2022 [7]. The Economist predicts that if Vietnam can maintain a 7% pace over the next decade, this nascent Asian Tiger will follow the same trajectory as South Korea and Taiwan [8].

Besides, recently there has been a series of major shocks to the global economy resulting from international and global events such as the US-China trade war, the pandemic, and the Russia-Ukraine war. Vietnam has proven itself to be a relatively safe and stable location for foreign investors. Consequently, Vietnam becomes vital link in supply chain as businesses pivot from China. The accelerating shift to countries such as Vietnam is part of a growing "China plus one" strategy to redraw global supply chains. As rivalries grow between China and the US over technology and security, more companies fear curbs on what and where they can manufacture [9] .

Nevertheless, despite successful growth rates in the last decades, Vietnam is still facing a

number of challenges in its efforts to sustain economic development and attract foreign investments, including bureaucracy and lack of transparency of the legal frameworks, infrastructure and transportation, and labor force.

Much has been discussed about legal and infrastructure issues. Regarding the labor force, Vietnam is currently enjoying a "golden population structure" that lasts for more than 30 years (from 2009 to 2039 in the case of Vietnam), that is, during such period working-age population (the population aged between 15 and 64) is about double the dependent population (people under age 15 and over age 64). Specifically, the percentage of the working-age population rose from around 56 % in 1986 to over 70 % in 2014 [10]. Thus, many studies have mentioned the great advantage of Vietnam with an "abundant labor force", "cheap labor" etc., since it was one of the important reasons to attract foreign investment and promote the development of labor-intensive manufacturing industries.

However, the main problem is that Vietnam's labor force has relatively low technical qualifications and lacks skills. The proportions of labor with professional and technical qualifications were 10% in 1999, 15.5% in 2009, 22.8% in 2018, and 26.1% in 2021 [11], showing a slow-moving improvement in labor quality compared to the economic growth rate and labor restructuring. Consequently, the labor productivity of Vietnam is not high. During the last two decades, although labor productivity growth increased rapidly, reaching an annual average of 4.77% from 2011 to 2018 (compared to 3.17% in 2007-2010), the productivity growth rate of Vietnam has always been lower than the economic growth rate. This shows the fact that current Vietnam’s economic growth is mainly based on expanding the production scale and utilizing more labor rather than based on labor productivity. Thus, in the era of knowledge and technology, it is essential to improve the quality of human resources by increasing the number of well-trained employees so that Vietnam can maintain economic growth and attract more foreign investments to avoid the "*middle-income trap*" and the risk of "*getting old before getting rich*" when the period of the "golden population structure" is over.

Vietnam has received the strong trend of foreign investment, but the question is whether the country has the infrastructure (both legal and physical) and adequate labor force to develop further.

Will Vietnam be able to imitate the success of past Asian Tigers?

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P10: Cocktail of REGN Antibodies Binds More Strongly to SARS-CoV-2 Than Its Components, But The Omicron Variant Reduces Its Neutralizing Ability

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Abstract

A promising approach to combat Covid-19 infections is the development of effective antiviral antibodies that target the SARS-CoV-2 spike protein. Understanding the structures and molecular mechanisms underlying the binding of antibodies to SARS-CoV-2 can contribute to quickly achieving this goal. Recently, a cocktail of REGN10987 and REGN10933 antibodies was shown to be an excellent candidate for the treatment of Covid-19. Here, using all-atom steered molecular dynamics and coarse-grain umbrella sampling we examine the interactions of the receptor binding domain (RBD) of the SARS-CoV-2 spike protein with REGN10987 and REGN10933 separately as well as together. Both computational methods show that REGN10933 binds to RBD more strongly than REGN10987. Importantly, the cocktail binds to RBD (simultaneous binding) more strongly than its components. The dissociation constants of REGN10987-RBD and REGN10933-RBD complexes calculated from the coarse-grained simulations are in good agreement with the experimental data. Thus, REGN10933 is probably a better candidate for treating Covid-19 than REGN10987, although the cocktail appears to neutralize the virus more efficiently than REGN10933 or REGN10987 alone. REGN10987's association with RBD is driven by van der Waals interactions, while the electrostatic interactions dominate in the case of REGN10933 and the cocktail. We also studied the effectiveness of these antibodies on the two most dangerous variants Delta and Omicron. Consistent with recent experimental reports, our results confirmed that the Omicron variant reduces the neutralizing activity of REGN10933,

REGN10987, and REGN10933+REGN10987 with the K417N, N440K, L484A, and Q498R mutations playing a decisive role, while the Delta variant slightly changes their activity.

Keywords: SARS-CoV-2, RBD, Covid-19, REGN-COV2, REGN10933, REGN10987, antibody cocktail, SMD simulation, Coarse-grained simulation, Delta variant, Omicron variant.

P11: SARS-CoV-2 Omicron Variant Binds to Human Cells More Strongly than Wild Type: Evidence from Molecular Dynamics Simulation

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Abstract

The emergence of the variant of concern Omicron (B.1.1.529) of the severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) aggravates the covid-19 pandemic due to its very contagious ability. The high infection rate may be due to the high binding affinity of Omicron to human cells, but both experimental and computational studies have yielded conflicting results on this issue. Some studies have shown that the Omicron variant binds to human angiotensin-converting enzyme 2 (hACE2) more strongly than wild type (WT), but other studies have reported comparable binding affinities. To shed light on this open problem, in this work, we calculated the binding free energy of the receptor binding domain (RBD) of the WT and Omicron spike protein to hACE2 using all-atom molecular dynamics simulation and molecular mechanics Poisson-Boltzmann surface area (MM-PBSA) method. We showed that Omicron binds to human cells more strongly than WT due to increased RBD charge, which enhances electrostatic interaction with negatively charged hACE2. N440K, T478K, E484A, Q493R and Q498R mutations in RBD have been found to play a critical role in the stability of the RBD-hACE2 complex. The effect of homogeneous and heterogeneous models of glycans coating the viral RBD and the peptidyl domain (PD) of hACE2 was examined. Although the total binding free energy is not sensitive to the glycan model, the distribution of per-residue interaction energies depends on it. In addition, glycans have little effect on the binding affinity of WT RBD to hACE2.

Keywords: Omicron variant, COVID-19, SARS-CoV-2, glycans, spike protein, human angiotensin-converting enzyme 2, receptor binding domain, peptidyl domain, MM-PBSA, binding free energy.

P12: Identifying Inhibitors of NSP16-NSP10 of SARS-CoV-2 from Large Databases

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Abstract

The COVID-19 pandemic, which has already claimed millions of lives, continues to pose a serious threat to human health, requiring the development of new effective drugs. Non-structural proteins of SARS-CoV-2 play an important role in viral replication and infection. Among them, NSP16 (non-structured protein 16) and its cofactor NSP10 (non-structured protein 10) perform C2'-O methylation at the 5' end of the viral RNA, which promotes efficient virus replication. Therefore, the NSP16-NSP10 complex becomes an attractive target for drug development. Using a multi-step virtual screening protocol which includes Lipinski's rule, docking, steered molecular dynamics and umbrella sampling, we searched for potential inhibitors from the PubChem and anti-HIV databases. It has been shown that CID 135566620 compound from PubChem is the best candidate with an inhibition constant in the sub-μM range. The Van der Waals interaction was found to be more important than the electrostatic interaction in the binding affinity of this compound to NSP16-NSP10. Further *in vitro* and *in vivo* studies are needed to test the activity of the identified compound against COVID-19.

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P13: Impact of Tourism on the Lives of Local People in A Luoi District, Thua Thien Hue Province (Vietnam)

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Abstract

A Luoi district tourism has been increasingly developing in recent years. This has greatly impacted the lives of local people in A Luoi district, including: economy, society and environment. Positive impacts, such as contributing to the economy of A Luoi district; People's income, spiritual life, and cultural level are improved; create many jobs; The relationship between family and the community becomes closer and more connected; Environmental protection and forest resource protection issues are given priority. However, there are some negative impacts such as people's income being increased but not yet large; Social evils have increased compared to before; The amount of solid waste during the tourist season increases dramatically, causing negative impacts on the environment; Natural landscapes have been renovated, water and air quality are adversely affected during peak days.

Keywords: A Luoi, tourism, people's lives, income, jobs, environment