

XXIst RENCONTRES DU VIETNAM | UNESCO'S OFFICIAL PARTNER
Gặp gỡ Việt Nam lần thứ 21 | Đối tác chính thức của UNESCO



THE THIRD INTERNATIONAL SYMPOSIUM OF NANO LIFE SCIENCE:
**NANO BIOTECHNOLOGY,
BIOPHYSICS, COMPUTATION**

HỘI THẢO QUỐC TẾ LẦN THỨ 3 VỀ KHOA HỌC SỰ SỐNG NANO:
CÔNG NGHỆ NANO SINH HỌC, LÝ SINH, TÍNH TOÁN

**ABSTRACT
BOOK 3rd**

 **September 17 - 19, 2025**

 **Quy Nhon, Vietnam**

SPONSORS/ORGANIZERS

NanoBioCoM2025 is organized and supported by Rencontres du Vietnam, International Centre for Interdisciplinary Science and Education (ICISE), Nano Life Science Institute-Kanazawa University, ADGROUP, Phenikaa University, and other institutions and Universities.



Welcome Message from the Organizing Committee of NanoBioCoM2025

Dear Colleagues and Participants,

On behalf of the Organizing Committee, we extend our warmest welcome to the XXIst Rencontres du Vietnam: The Third International Symposium on Nano Life Science: Nano Biotechnology, Biophysics, and Computation (NanoBioCoM2025).

We are thrilled to host this gathering of brilliant minds from across the globe. This symposium is dedicated to the vibrant and interdisciplinary frontiers of nanobiotechnology, biophysics, and computational modeling - fields that are redefining our understanding of life itself.

NanoBioCoM2025 is designed to be more than just a conference; it is a catalyst for collaboration. Our program features plenary lectures by world-renowned scientists, invited and keynote talks, oral and poster presentations, and dedicated panels on education and international research partnerships. This symposium is particularly special for the biophysics community right here in Vietnam. We are a young community fueled by incredible passion and talent, eager to contribute to the global scientific dialogue. NanoBioCoM2025 serves as a vital platform for our local researchers to connect with the global research landscape.

We encourage you to immerse yourself in scientific dialogue, forge new connections, and explore potential collaborations. Your active participation is the key to a successful and inspiring event.

We look forward to sharing not only groundbreaking science but also the unique atmosphere of the ICISE Center in the beautiful city of Quy Nhon. We are confident this setting will provide the perfect backdrop for thoughtful discussion and fruitful exchange.

Thank you for being a part of NanoBioCoM2025.

With warm regards,

The Organizing Committee

NanoBioCoM2025

September 17-19, 2025, ICISE, Quy Nhon, Vietnam



Nguyen The Toan

Chairman



Tran Quang Huy

Co-Chairman



Bui Khanh Huy

Co-Chairman

Preface

Over the last few years, artificial intelligence and breakthroughs in advanced techniques have changed the research landscape significantly. This symposium is designed to navigate this change. We focus on biophysics, the field where physics and biology meet to reveal the physical mechanisms of life. A central challenge is resolving the gap between single-molecule and ensemble experiments. This is key to true understanding in nano life science.

This year's meeting is our most international meeting yet. We also received 55 abstracts for plenary, keynote, invited, oral and 42 for poster presentations. Scientists from 13 countries gathered in Quy Nhon to share their work. They came from Vietnam, Japan, France, Germany, UK, Russia, Australia, Kazakhstan, Taiwan, Algeria, Canada, Malaysia, USA, and Korea. This diversity of thought is our greatest strength.

Our core aim remains: to bridge experimental and computational methods. We showcase everything from molecular dynamics to AI-driven deep learning to address fundamental questions. For Vietnam, a nation actively building its research future, this symposium is a catalyst. It connects our dynamic young community with world leaders to advance programs in nanomedicine, biosensing, and computational biology.

We would like to express our great appreciation to Prof. Jean Tran Thanh Van – President of Rencontres du Vietnam and Prof. Le Kim Ngoc for their generous support to this event. We are especially grateful to the WPI Nano Life Science Institute at Kanazawa University for their generous grant supporting women scientists. This award is a crucial step toward a more inclusive scientific future.

We thank all participants, the Rencontres du Vietnam, and our supporting institutions. We look forward to this symposium growing as a cornerstone event for international science in Vietnam.

The Organizing Committee

NanoBioCoM2025

September 2025

Establishment of the Vietnamese Biophysical Society (VBS)

The Vietnamese Biophysical Society (VBS) is a subdivision of the Vietnam Physical Society, serving as the national representative body for the advancement of education, research, and development in biophysics. Society was founded to connect scientists, lecturers, and students, while promoting academic exchange, enhancing the quality of training and research, and fostering the application of biophysical achievements in life sciences, medicine, agriculture, and technology.

VBS is the official representative of Vietnam in the International Union for Pure and Applied Biophysics (IUPAB) and maintains close collaborative relationships with regional and international biophysics societies. Through conferences, workshops, training programs, and joint research initiatives, VBS plays a vital role in integrating the Vietnamese biophysics community into the global scientific arena, while contributing to the sustainable development of science and technology in the country.

The idea of establishing VBS originated from a group of lecturers and scientists from Phenikaa University, Nong Lam University, the Military Medical Academy, Hue University, Vietnam National University, Hanoi Medical University, together with academic support from Kanazawa University (Japan). Driven by the urgent need to create a professional community for research collaboration and educational advancement, the founding group engaged in extensive discussions and preparations.

After a period of groundwork and advocacy, VBS was officially established in 2025 with broad consensus from research institutions and biophysics experts both within and outside Vietnam.

From its inception, VBS has set forth key strategic goals:

- To encourage fundamental and applied research in biophysics.
- To establish a forum for academic exchange, research collaboration, and the training of high-quality human resources.
- To promote scientific publications, including the future establishment of a specialized journal to disseminate research results.
- To support the development of policies and strategies for scientific and technological advancement in medicine, agriculture, environment, and biotechnology.

Among its prominent activities, VBS organizes national and international scientific conferences and workshops, as well as specialized training courses for lecturers and young researchers. The Society also actively participates in interdisciplinary projects and international collaborations, thereby enhancing Vietnam's scientific standing on the global stage.

With its mission to promote biophysical research, education, and applications, VBS is steadily affirming its pioneering role in connecting the scientific community, fostering international integration, and contributing to the sustainable development of science and technology in Vietnam.

Official website

<https://vietbiophysics.vn/>



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- **Ms. Nguyen Thi Thanh Loan** – ICISE Quy Nhon, Vietnam

DETAILED AGENDA

DAY 1		
Wednesday, September 17, 2025		
7:45 – 8:15	Moving to ICISE from Seagull Hotel by Shuttle Buses	
8:30 – 9:00	Registration	
9:00 – 9:45	Opening ceremony - Welcome speech by Prof. Jean Tran Thanh Van (ICISE) - Speech by a Representative of GiaLai Province - Opening speech by Prof. Nguyen The Toan, Chairman of NanoBioCoM2025 - Speech by Prof. Nguyen Quang Liem, President of Vietnam Physical Society (VPS) - Launching the Vietnamese Biophysical Society (VBS) – Introduction of Provisional Executive Committee - Group photo	
9:45 – 10:00	Coffee break	
	PLENARY SESSION, HALL 1 Chairs: Prof. Nguyen Quang Liem and Prof. Takeharu Nagai	
10:00 – 10:40	PL-01: Theoretical physics and the challenge of modern biology: a personal perspective	Prof. Dr. Curtis Callan Princeton University, USA
10:40 – 11:10	K-01: Expanding the Frontiers of Autonomous Bioluminescence: Multicolor Variants and Applications for Life Science	Prof. Dr. Takeharu Nagai The University of Osaka, Japan
11:10 – 11:40	K-02: Computation with AFM data: Imaging and structural biology; Nano-indenting and plant biology	Dr. Jean-Luc PELLEQUER Institut de Biologie Structurale, France
11:40 – 12:10	K-03: Functional Extensions of High-Speed AFM for Probing Nanomechanical Dynamics in Live Cells	Prof. Dr Takayuki Uchihashi Nagoya University, Japan
12:10 – 13:30	Lunch	

	PLENARY SESSION, HALL 1 Chairs: Prof. Nguyen The Toan and Assoc. Prof. Bui Khanh Huy	
13:30 – 14:00	K-04: Influx-dependent Local Ca²⁺ Increases Regulate Myosin II and Myosin VI: Activation to Promote Rupture of the Shigella-Containing Vacuole	Prof.Dr Guy Tran Van Nhieu University of Paris Saclay, France
14:00 – 14:30	K-05: Aptamer-Based Rapid Detection of Biomarkers in Infectious Diseases and Cancer	Assoc. Prof. Damira Kanayeva, Nazarbayev University, Kazakhstan
14:30 – 15:00	K-06: Single-cell analysis using glass nanopipette-based scanning probe microscopy	Prof. Dr. Yasufumi Takahashi NanoLSI, Kanazawa University, Japan
15:00 – 15:40 (Online)	PL-02: The Importance of Water in Biology – An Example of Receptor Function and Its Implications for Optogenetics	Prof. Dr. Anthony Watts University of Oxford, UK
15:40 – 16:00	Coffee break	
	PARALLEL SESSIONS	
	Session 1: Nano Biotechnology (HALL 1) Chairs: Assist. Prof. Pham Thanh Tri, Assoc.Prof.Dr Nguyen Thi Thu Hoai	Session 2: Biophysics and Computation (HALL 2, 2 nd floor) Chairs: Assoc. Prof. Bui Khanh Huy, Dr. Van Ngo
16:00 – 16:25	IN-01: Protein engineering for genetically encoded biosensors to visualize cellular metabolism in living tissue Assist.Prof.Dr. Yusuke Nasu Institute of Biological Chemistry, Academia Sinica, Taipei, Taiwan	IB-01: Thermogenetic toolkit for controlling cellular function Assist. Prof. Dr Cong Quang Vu WPI Nano Life Science Institute, Kanazawa University, Japan

16:25 – 16:50	IN-02: Applications of photonic micro and nanostructures in optical biosensors and microbiolasers Assoc.Prof.Dr. Mai Hong Hanh University of Engineering and Technology, VNU Hanoi	IB-02: Multiscale AFM Investigation of CRMP2-Microtubule Interactions and Impact on Glioblastoma Cell Mechanics Assist. Prof.Dr. Djamel Eddine Chafai, WPI Nano Life Science Institute, Kanazawa University, Japan
16:50 – 17:15	IN-03: Enhanced Dengue Virus Detection and Quantification Using a CRISPR-Cas13a-Lipid Droplet Integrated Assay Assoc.Prof.Dr Nguyen Thi Thu Hoai School of Biotechnology and Research Center for Infectious Diseases, International University, National University Ho Chi Minh City, Vietnam	IB-03: How biomechanics shapes plant organs Dr. Duy-Chi Trinh University of Science and Technology of Hanoi, Hanoi, Vietnam
17:15 – 17:40	IN-04: Plasma-Assisted Fabrication of Dual Optical Nanomaterials for High-Sensitivity Detection of Aflatoxin B1 Dr. Nguyen Minh Hoa University of Medicine and Pharmacy, Hue University, Vietnam	IB-04: Translation dynamics and impact of ribosome structure at the nanoscale Assist. Prof. Dr Dao Khanh Duc University of British Columbia, Canada
17:40 – 18:05	IN-05: Development of SERS Substrates Using Nanostructured Semiconductors and Metal Nanoparticles for Pharmaceutical Detection Dr. Le Thi Minh Huyen University of Medicine and Pharmacy at HoChiMinh City	IB-05: Shear-induced fibronectin fibrillogenesis: Differential mechanisms under high and low shear stress conditions Assoc. Prof.Dr Huynh Chan Khon International University, Vietnam National University, HCMC, Vietnam

18:05 – 18:25	O-01: Application of Atomic Force Microscopy in Materials Science and Cosmetics: Exploring the nanostructural, mechanical and chemical properties Dr. Tran Thi Quynh Université Paris-Saclay, CNRS, Institut de Chimie Physique, UMR 8000, 91405 Orsay, France	O-02: The Role of Entropy Production and Spectral Gaps in Giant Diffusion Dr. Vo Van Tuan Kyoto University, Japan
18:30 - 19:30	Dinner at ICISE	
19:30	Moving to hotels by shutter buses, free excursion	
DAY 2 Thursday, September 18, 2025		
8:15 – 9:00	Moving to ICISE from Seagull Hotel by Shuttle Buses, and hanging posters	
	PLENARY SESSION, HALL 1 Chairs: Prof. Erik Schäffer and Assoc. Prof. Dr. Tran Quang Huy	
9:00 – 9:30 (Online)	K-07: Micro Elastofluidics: Elasticity and Flexibility for Efficient Microscale Liquid Handling	Prof. Nam-Trung Nguyen Queensland Quantum and Advanced Technologies Research Institute, Griffith University, Australia
9:30 – 10:00	K-08: Pushing Optical Tweezers Limits: How Kinesins Walk - It’s Not How You Thought!	Prof.Dr. Erik Schäffer University of Tübingen, Germany
10:00 – 10:30	K-09: Multiple Mechanisms to Regulate Actin Functions: “Fundamental” versus Lineage-Specific Mechanisms	Prof. Taro Uyeda Waseda University, Japan
10:30 – 11:00	Coffee break	

	PLENARY SESSION, HALL 1 Chairs: Assoc. Prof. Damira Kanayeva and Assoc. Prof. Dao Khanh Duc	
11:00 – 11:30	K-10: Unlocking Hidden Local Protein Dynamics with Temporal Resolution Using Geometric Descriptors for Nuclear Receptor in Silico Biophysics	Assoc.Prof.Dr Ferdinand Molnar Nazarbayev University, Kazakhstan
11:30 – 12:00	K-11: Design Lipid Nano Carriers Based on Their Interfacial Properties	Prof. Dr. Hiroshi Umakoshi Osaka University, Japan
12:00 – 13:30	Lunch	
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	Session 1: Nano Biotechnology (HALL 1) Chairs: Assist. Prof.Dr. Kee Siang, Lim and Assoc. Prof. Nguyen Hoang Anh	Session 2: Biophysics and Computation (HALL 2, 2 nd floor) Chairs: Prof. Tran Van Hieu, Assist.Prof.Dr. Djamel Eddine Chafai
13:30 – 13:55	IN-06: Nanoscopic Exploration of the Journey to the Nucleus Assist. Prof.Dr. Kee Siang Lim WPI Nano Life Science Institute, Kanazawa University, Japan	IB-06: Atomic Conformational Dynamics and Actin-Crosslinking Function of Alpha-Actinin Revealed by SimHS-AFMfit Assist. Prof. Dr. Kien Xuan Ngo WPI-NanoLSI, Kanazawa University, Japan
13:55 – 14:20	IN-07: Prebiotic oligosaccharides resembling human milk oligosaccharides: from enzyme production to enzymatic synthesis Assoc. Prof. Dr. Nguyen Hoang Anh Vietnam National University of Agriculture, Hanoi, Vietnam	IB-07: Large Scale Simulations of Highly Flexible and Dynamical Proteins in Cellular Signaling Dr. Van Ngo Oak Ridge National Laboratory, USA

14:20 – 14:40	O-03: Preparation, Characterization, and Evaluation of Silver Nanoparticles from Allium cepa <i>L. Peel</i> Extract Dr. B. Samuel Thavamani Dept. of Pharmacognosy, Ahalia School of Pharmacy, Kerala, India	IB-08: M cells or not to M cells: an update Prof.Dr. Tran Van Hieu Faculty of Biology and Biotechnology University of Science, VNU-HCM
14:40 – 15:00	O-04: Advanced biosynthesis to boost the production of natural antibiotics for antimicrobial applications Ms. Malika Toleubekova Nazarbayev University, Kazakhstan	O-05: Application of coarse-grained DNA mathematical model for studying the genesis of additional open state zones in the extended polyQ tract of the ATXN2 gene Prof.Dr. Stepan Dzhimak Kuban State University, Krasnodar, Russian Federation
15:00 – 15:20	O-06: Biosynthesis and characterisation of Silver nanoparticles using <i>Bacillus.subtilis</i> and their commercial formulation Bensam Manuel S Karunya Institute of Technology and Sciences, Coimbatore, Tamil Nadu, India	O-07: Engineering small modular recombinant antibodies for chromatin studies Ms. Pham Thi Huong Quynh Nano Life Science Institute, Kanazawa University, Japan
15:20 – 15:40	Coffee Break	
	PLENARY SESSION, HALL 2	
15:40 – 16:40	Poster presentation	
16:40 – 17:50	1st Meeting of Vietnamese Biophysical Society	
18:00 – 21:30	Cocktails and Gala Dinner	
21:30	Moving to hotels by shutter buses	

DAY 3 Friday, September 19, 2025		
8:30 – 9:00	Moving to ICISE from Seagull Hotel by Shuttle Buses	
	PLENARY SESSION, HALL 1 Chairs: Assoc.Prof. Ferdinand Molnar, Assist.Prof. Yusuke Nasu	
9:00 – 9:30	K-12: Deciphering Ciliary Assembly: Insights Revealed by Cilia Tip Structure	Assoc. Prof. Dr. Khanh Huy Bui Department of Anatomy and Cell Biology, McGill University, Montreal, Quebec, Canada
9:30 – 10:00	K-13: <i>Drosophila melanogaster</i> as a rapid, reliable and cost-effective platform for assessing the efficacy of drugs and nanoparticles	Assist. Prof. Dr. Tri Thanh Pham Department of Biology, School of Sciences and Humanities, Nazarbayev University, Kazakhstan
10:00 – 10:30	K-14: Physics insights in a comprehensive drug design pipeline at the Key Laboratory for Multiscale simulation of complex systems	Prof.Dr. Nguyen The Toan Hanoi University of Science, VNU-Hanoi
10:30 – 10:55 (Online)	IN-08: Enhanced delivery of nanomedicines by Au nanoparticles	Assoc. Prof. Dr. Anh T.N. DAO Graduate School of Integrated Science and Technology, Nagasaki University, Japan
10:55 – 11:00	Coffee break	
	PARALLEL SESSIONS	
	Session 1: Nano Biotechnology (HALL 1) Chairs: Prof. Nguyen Kim Nga and Dr. Nguyen Ba Hung	Session 2: Biophysics and Computation (HALL 2, 2 nd floor) Chairs: Dr. Cong Quang Vu and Assoc.Prof. Tran Thi Thu Hanh

11:00 – 11:25	IN-09: Bioceramics and 3D scaffolds for bone tissue engineering Prof. Dr Nguyen Kim Nga School of Chemistry and Life Science, Hanoi University of Science and Technology, Vietnam	IB-09: Decoding Gene Regulation Mechanisms and Target Cancer-Causing Proteins Dr. Trinh Bon University of Virginia School of Medicine, USA
11:25 – 11:50	IN-10: Fabrication of magnetically separable magnetite - graphene hybrid materials with enhanced photocatalytic efficiency for dye degradation Dr. Nguyen Ba Hung Vietnam Military Medical University, Hanoi, Vietnam	IB-10: Docking and Molecular Dynamics Study of Silk Fibroin Interactions with Carbon Nanotube Assoc.Prof. Dr. Tran Thi Thu Hanh Ho Chi Minh City University of Technology (HCMUT), VNU-HCM, Ho Chi Minh, Vietnam
11:50 – 12:15	IN-11: Electrochemical sensors for trace level detection of heavy metal ions in water by modification of micro electrodes with nano-structured composite layers Assoc. Prof. Doan Duc Chanh Tin Institute for Nanotechnology – Vietnam National University, Ho Chi Minh City	IB-11: Cancer detection and classification utilizing polarized/medical images and artificial intelligence (AI) models Assoc.Prof. Pham Thi Thu Hien International University, Vietnam National University, HCMC, Vietnam
12:15 – 12:35	O-08: Enhanced Superconductivity in Pb₂Au Alloy on Pb (111) Ms Huynh Truc Nhu National Tsing Hua University, Taiwan	O-09: From UV Activation to Surface Binding: Charge Transfer Strategies in SERS Ms Dao Thi Nguyet Nga Phenikaa University Nano Institute, Phenikaa University, Hanoi, Vietnam
12:35 – 13:30	Lunch	
13:30 – 14:30	Poster presentation	

	PLENARY SESSION, HALL 1 Chairs: Prof. Dr. Takayuki Uchihashi and Dr. Van Ngo	
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15:00 – 15:25 (Online)	IB-12: Structures and Dynamics of Large RNA Molecules Explored with Coarse-Grained Simulations	Assit. Prof. Naoto Hori University of Nottingham, UK
15:25 – 15:55 (Online)	K-16: Learning Protein Motions	Prof. Dr. Sergei Grudinin Grenoble Alpes University, France
15:55 – 16:25 (Online)	K-17: Design of Bimodal Carbon Dots for Dual-Mode MRI and CT Contrast Imaging	Assoc.Prof. Timur Atabaev Nazarbayev University, Kazakhstan
16:25–16:45	O-11: Influence of Surface Chemistry on the Toxicity of Thiolated and PEGylated Organosilica Nanoparticles	Balnur Zhaisanbayeva Nazarbayev University, Kazakhstan
16:45–17:05	O-12: Myco-engineered silver nanoparticles from <i>Penicillium oxalicum</i> exhibits <i>in vitro</i> anti-proliferative activity and potentially mediates <i>in vivo</i> breast tumor regression	Priyamvada Gupta Banaras Hindu University, India
17:05 – 17:30	Coffee break	
17:30 – 18:00	Poster awards and Closing ceremony	
18:00 - 19:30	Dinner at ICISE	
19:30	Moving to Seagull Hotel by Shuttle Buses/ Free Excursion	
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	⁴ <i>Tufts Stuart B Levy Center for Integrated Management of Antimicrobial Resistance, Tufts University, Boston, MA, 02111, USA</i>	
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PP-32	Preparation of gold nanoparticles stabilized in water-soluble β-glucan by gamma irradiation with high antioxidant and anticancer activities Nguyen Trong Nghia^{1,2}, Do Thi Phuong Linh^{2,3}, Nguyen Thanh Vu¹, Nguyen Thi Ngoc Anh¹, Lam Vy Nguyen², Nguyen Vu Phong², Le Quang Luan^{1*} ¹ <i>Department of Biomaterial and Nano Technology, Biotechnology Center of Ho Chi Minh City, Ho Chi Minh City 700000, Vietnam;</i> ²<i>Faculty of Biological Science, Nong Lam University, Ho Chi Minh City 700000, Vietnam;</i> ³ <i>Institute of Malariology Parasitology and Entomology in Ho Chi Minh City, Ho Chi Minh City 700000, Vietnam;</i>	136

PP-33	Fabrication of Fluorescent PDMS/RhB Microspheres for Antibody Purification Applications Luong Thi Phuong Thao¹, Luu Manh Quynh², Pham Xuan Thao³, Kieu Bao My¹ ¹ Faculty of Biology, University of Science, Vietnam National University, Hanoi, Vietnam ² Faculty of Physic, University of Science, Vietnam National University, Hanoi, Vietnam ³ Faculty of Fundamental Science, Hanoi University of Industry, Hanoi, Vietnam	137
PP-34	Study on the fabrication of nanobody conjugated amine-magnetic particles for the purification of botulinum toxin type A light chain My Bao Kieu¹, Quynh Manh Luu², Nhung Thi Hong Le^{1,3} ¹ Faculty of Biology, VNU University of Science, Hanoi, Vietnam, 334 Nguyen Trai, Thanh Xuan, Ha Noi, Vietnam ² The Faculty of Physics, VNU University of Science, Hanoi, Vietnam, 334 Nguyen Trai, Thanh Xuan, Ha Noi, Vietnam ³ Key Laboratory of Enzyme and Protein Technology, VNU University of Science, Hanoi, Vietnam, 334 Nguyen Trai, Thanh Xuan, Ha Noi, Vietnam	139
PP-35	Temperature-modulated toxicity of bisphenol A in zebrafish (<i>Danio rerio</i>) embryos: morphological, physiological, and transgenerational responses Pham Thi Quyen¹, Tran Anh Duc¹, Kieu Trung Kien¹, Dr. Pham Thi Thu Huong², Dr. Pham Thi Dau^{1,3} ¹ Deparment of Biology, VNU University of Science, 334 Nguyen Trai, Hanoi, Vietnam ² Key Laboratory of Enzyme and Protein Technology, VNU University of Science, 334 Nguyen Trai, Hanoi, Vietnam ³ Center for Life Sciences Research, VNU University of Science, 334 Nguyen Trai, Hanoi, Vietnam	140
PP-36	Non-invasive prediction of colorectal cancer using an ensemble stacking model based on circulating mRNA Ngoc Hai Ngo¹, Thanh Dat Nguyen², Tung Minh Ly³, Thi My Hanh Pham⁴, Minh Nam Nguyen^{2,3*} ¹ Nong Lam University Ho Chi Minh City ² Research Center for Genetics and Reproductive Health, School of Medicine, Vietnam National University Ho Chi Minh City ³ Faculty of Medicine, University of Health Sciences, Vietnam National University Ho Chi Minh City ⁴ University of Science, Vietnam National University Ho Chi Minh City	141
PP-37	Toward enhanced bioavailability and controlled release of poorly soluble drugs by room-temperature atomic layer deposition: a case study of gliclazide Diem-Quyen T. Nguyen¹, Viet Phuong Ca², Truong Duc Dinh², Tuan Hiep Tran³, Hao Van Bui² ¹ Faculty of Fundamental Sciences, Phenikaa University, Duong Noi, Hanoi 12116,	142

	<i>Vietnam</i> ²<i>Faculty of Materials Science and Engineering, Phenikaa University, Duong Noi, Hanoi 12116, Vietnam</i> ³<i>Faculty of Pharmacy, Phenikaa University, Duong Noi, Hanoi 12116, Vietnam</i>	
PP-38	Stable dispersion and prolonged dissolution of hydrophilic pharmaceutical achieved by room-temperature atmospheric pressure atomic layer deposition Cao Viet Phuong¹, Kim-Hue Thi Dinh¹, Truong Duc Dinh¹, Phi Huu Bui¹, Tuan Hiep Tran², Hao Van Bui^{* 1} ¹<i>Faculty of Materials Science and Engineering, Phenikaa University, Yen Nghia, Ha Dong District Hanoi 12116, Vietnam</i> ²<i>Faculty of Pharmacy, Phenikaa University, Yen Nghia, Ha Dong District Hanoi 12116, Vietnam</i>	143
PP-39	Molecular Dynamic Simulation Study of Deformation Behavior and the Role of Chitosan in Reinforcing Bombyx mori Fibroin Composites Under Acidic Conditions Phuc Vu Le^{1,2}, Duy Phuoc Tran³, Hanh Thi-Thu Tran^{1,2,*} ^{1,2}<i>Biomedical Engineering Physics Department, Faculty of Applied Science, Ho Chi Minh City University of Technology (HCMUT), VNU-HCM, Ho Chi Minh City, Vietnam.</i> ³<i>School of Life Sciences and Technology, Tokyo Institute of Technology, Japan</i>	144
PP-40	Density Functional Theory Perspective On Single – Atom Fe/N-Embedded Graphdiyne As An Efficient Electrocatalysts For The Hydrogen Evolution Reaction Tan Phat Pham¹, Minh Tam Le¹, Minh Dang Le¹, Nguyet N. T. Pham^{1,2,*} ¹<i>University of Science, Vietnam National University, 227 Nguyen Van Cu, Ho Chi Minh City 700000, Vietnam</i> ²<i>Vietnam National University, Ho Chi Minh City (VNU-HCM), Vietnam.</i>	145
PP-41	Access to Functionalized α,β-Unsaturated Imines through Bicyclic Ketone Intermediates Nguyen Thu Ha (student) <i>Faculty of Chemistry, VNU - University of Science</i>	146
PP-42	Lipid–Gold nanoparticles–Curcumin Conjugates as Plasmon-Enhanced Antimicrobials Against Multidrug-Resistant <i>Escherichia coli</i> Nguyen Thi Bich¹, Nguyen Thi Hue², Nguyen Thi Thu Thuy¹, Tran Quang Huy^{1,2,*} ¹<i>Phenikaa University Nano Institute, Phenikaa University, Hanoi, Vietnam</i> ²<i>Faculty of Biomedical Sciences, Phenikaa School of Medicine and Pharmacy, Phenikaa University, Hanoi, Vietnam.</i>	147

PLENARY LECTURES

PL-01 Theoretical physics and the challenge of modern biology: a personal perspective

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Modern physics and modern biology have a common problem: the data they can collect is often too copious and indirect to mean anything without a mathematical framework on which to hang the data. Constructing such frameworks for the inanimate world is of course the task of theoretical physics. Some theoretical physicists have wondered whether a similar approach might be brought to bear on the flood of data being collected in life sciences. I will try to illustrate what such an effort might look like by telling a couple of stories about my own efforts in this direction.

PL-02 The Importance of Water in Biology – An Example of Receptor Function and Its Implications for Optogenetics

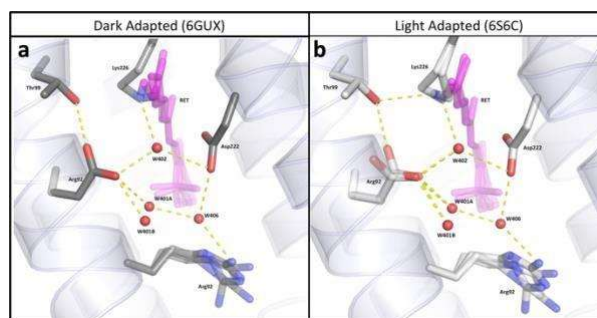
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Resolving conformational changes in membrane receptors in response to a stimulus, and capturing their functionally relevant dynamics, is very challenging. Over the years we have addressed this challenge using a range of spectroscopic approaches^{1,2,3} on functionally competent photoreceptors, often in their natural membranes⁴ or LipodisqsTM⁵. More recently, we have complemented this work with functional studies, mass spec characterization⁶ and very high resolution (1.07Å) crystallography^{7,8}, as well as photo- induced x-ray, free electron laser studies

(XFELS), without the use of detergents and including natural lipids. This high-resolution information reveals waters and their importance in both receptor activation- desensitization and QM(SCC-DFTB)/MM MD trajectories give information about the activation process. The system studied is achearhodopsin-3 (AR3), a photoreceptor utilized widely in optogenetics despite the



lack of structures until now. We suggest that the different arrangement of internal water networks in AR3 is responsible for the faster photocycle kinetics compared to homologs – AR3 is ~10x more efficient than bacteriorhodopsin at current generation. These insights may well have generic implications for other receptors.

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KEYNOTE LECTURES

K-01 Expanding the Frontiers of Autonomous Bioluminescence: Multicolor Variants and Applications for Life Science

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Abstract: Bioluminescence imaging has become an indispensable technology in modern biological research, offering high sensitivity, a wide dynamic range, and the ability to visualize cellular processes in living systems with minimal phototoxicity and negligible excitation-induced background. Yet conventional approaches are fundamentally constrained by their reliance on exogenously supplied substrates such as luciferin. Because these substrates are gradually consumed and can distribute unevenly in tissues, signal intensities decay over time and spatial uniformity is compromised, complicating long-term, quantitative imaging—particularly in three-dimensional samples and extended time-lapse experiments.

To address these limitations, genetically encoded autonomous bioluminescence systems have emerged. Two natural paradigms, the bacterial *lux* system and the fungal *luz* system, comprise gene clusters that encode both the light-emitting proteins and the biosynthetic enzymes required to produce the luminescent substrate in situ. When the complete set of essential genes is introduced into host cells, tissues, or organisms, the engineered system becomes self-sustained: samples glow continuously without exogenous luciferin, enabling stable imaging over long durations with inherently low background.

In this symposium, I will introduce our recent achievement regarding successful development of multi-color variants of autoluminescent proteins as well as their application to subcellular localization tags, multiple gene reporters, and Ca²⁺ dynamics at the single-cell level.

Keywords: *Autonomous bioluminescence, Multicolor imaging, Bioluminescent proteins, Gene reporters, Lux system, Luz system*

K-02 Computation with AFM data: Imaging and structural biology; Nano-indenting and plant biology

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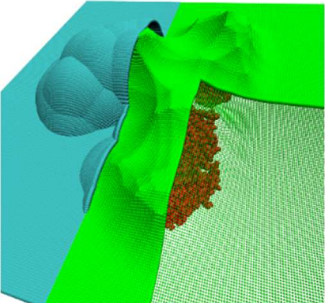
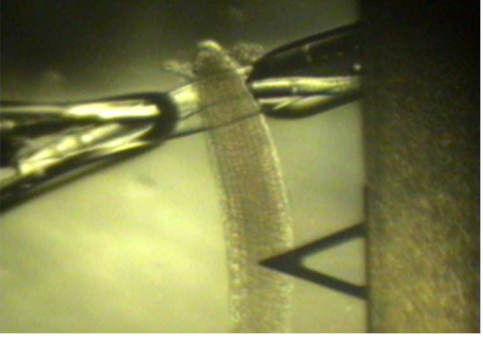
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Abstract: The Atomic Force Microscope (AFM), first described in 1986, is a rare mesoscopic biophysical tool. Depending on the experimental setup, it can observe the topography of isolated objects ranging from the electron cloud ($\sim \text{\AA}$) to molecules (nm), individual cells (μm), and tissues (mm). In addition to topography, the AFM can measure the stiffness of soft- or bio-materials, shedding new light on the mechanical properties of biological functions. In this presentation, we will discuss two topics in which AFM data is at the core of these measurements: imaging and nano-indenting.

Despite the widespread use of integrated structural biology, the combination of multi-source and multi-scale experimental data to determine the three-dimensional structure of a system, the use of AFM data remains limited, primarily due to the challenges of converting topography data into useful structural biology information. The first part of the presentation will introduce our strategy for incorporating AFM topography data into structural biology using the AFM-Assembly pipeline [1-3]. This pipeline takes as input a topographic map derived from high-resolution AFM imaging and structural units obtained from the Protein Data Bank and fits these atomic coordinates beneath the surface of the topographic surface. We will describe how static images can produce dynamical information on protein structures.

Recently, we performed nanoindentation experiments on 4-day-old living roots of *Arabidopsis thaliana* [4]. We observed that the external primary cell wall of the root stiffened and exhibited a root growth-arrest phenotype when the root was grown under low phosphate conditions. However, classical approaches for determining the stiffness of these root tissues are limited by the non-homogeneity of the plant root structure. We developed a novel, simpler strategy to estimate the stiffness of plant roots using the trimechanics framework [5]. I will describe its theoretical background and its application to measuring the stiffness of plant roots under abiotic metallic stress [6-7].

These two examples illustrate the vast power of AFM data operation beyond pretty pictures and Young's modulus. As these examples demonstrate, there is a great need for methodological development regarding AFM data. The golden age of AFM has yet to come.

	
One of the challenges associated with AFM topography is illustrated by the erosion process required to correct the tip-effect surface (cyan) to produce a refined topographic surface (green) above the isolated molecule (red spheres).	Root tip of an <i>Arabidopsis thaliana</i> seedling fixed on a glass slide using a silicon-based pressure-sensitive adhesive. The triangular shape of a PNP cantilever is located near the root transition zone, approximately 500 μm away from the root tip.

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K-03 Functional Extensions of High-Speed AFM for Probing Nanomechanical Dynamics in Live Cells

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Abstract: The advent of high-speed atomic force microscopy (HS-AFM) has paved the way for a new era in life sciences by enabling the direct, real-time observation of biomolecules in action, which were previously understood only as static structures. Dynamic processes of various proteins have been captured with sub-second temporal resolution, revealing the dynamics of biomolecules in aqueous environments that cannot be captured by X-ray crystallography or cryo-electron microscopy.¹⁾

As a next step beyond topographic imaging, we have focused on functional extensions such as correlative imaging and the simultaneous measurement of physical properties like mechanical characteristics. For correlative measurements, the development of a tip-scanning HS-AFM system has enabled integration with fluorescence microscopy²⁾, making it possible to simultaneously perform fluorescence and HS-AFM observations on the same sample. Furthermore, leveraging the advantage of a stationary sample stage in this setup, this platform has been extended to other types of functional enhancements, such as applying physical forces to the sample by stretching or compressing the substrate. This has enabled new research in mechanobiology, such as exploring the influence of membrane curvature on protein behavior.³⁾

For physical property measurements, what decisively distinguishes AFM from other high-resolution techniques is its ability to directly interact with the sample via its probe. This feature allows for the manipulation of the sample and the measurement of quantitative mechanical properties, such as stiffness (elastic modulus). In biological systems, mechanical properties play a crucial role in cell fate determination and tissue morphogenesis. Combining this unique mechanical approach of AFM with high-speed capabilities opens up a new research frontier: capturing the dynamic changes in mechanical properties associated with biological phenomena in real-time. We have developed a new technique, high-speed in-line force mapping (HS-iFM)⁴⁾ and

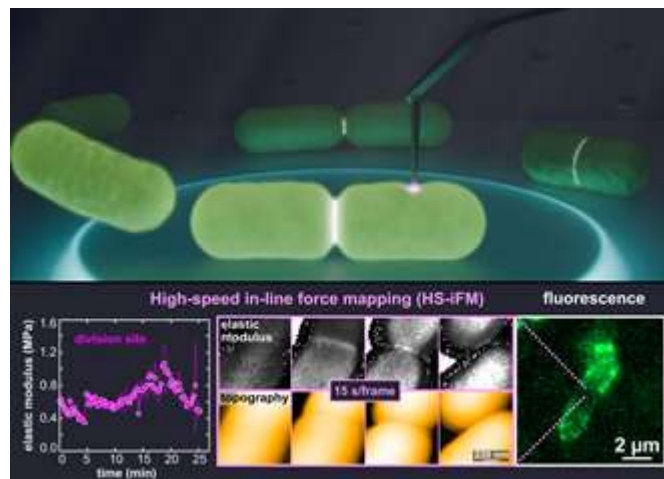


Figure: Overview of *E. coli* observation using HS-iFM. (Top panel) A schematic of *E. coli* observation by HS-iFM. (Bottom panel) A graph showing the stiffness change of *E. coli* measured by HS-iFM (left), time-lapse HS-iFM images of *E. coli* (center), and a fluorescence image of *E. coli* (right).

have succeeded in visualizing the dynamic changes in mechanical properties during the cell division of living *E. coli* with unprecedented spatiotemporal resolution. This technique can simultaneously acquire topography and elastic modulus maps at frame times as fast as 15 seconds. As a result, we successfully captured the dynamic changes in elastic modulus during the *E. coli* division process, such as the transient stiffening of the division site and the contribution of internal pressure to stiffness (Fig. 1).

Thus, the functional extensions of HS-AFM provide powerful tools not only to "see" biological phenomena but also to "measure and understand" the underlying mechanical mechanisms. In this presentation, I will introduce the technological developments and applications of these HS-AFM functional extensions and discuss the new horizons in the life sciences unveiled by this technology.

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- 4) C. Ganser *et al*, "A look beyond topography: Transient phenomena of Escherichia coli cell division captured with high-speed in-line force mapping", *Sci. Adv.* **11**, eads3010 (2025).

Keywords: HS-AFM, Correlative Imaging, HS-iFM, Quantitative Nanomechanics, Mechanobiology

K-04 Influx-dependent Local Ca²⁺ Increases Regulate Myosin II and Myosin VI Activation to Promote Rupture of the *Shigella*-Containing Vacuole

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Abstract: *Shigella*, the causative agent of bacillary dysentery, invades epithelial cells to colonize the intestinal mucosa. During *Shigella* invasion, an actin coat forms around the bacteria containing vacuole, preceding vacuolar rupture and bacterial escape and replication in the cell cytosol. While critical for virulence and the subsequent bacterial infection steps, the process by which *Shigella* ruptures the phagocytic vacuole is poorly understood. Recent studies point to a role of trafficking, including sorting and recycling pathways in vacuolar rupture, but how these promote vacuolar rupture remains unclear. We show here that rupture of the *Shigella* vacuole requires Ca²⁺ influx and is associated with long lasting local Ca²⁺ increases. Influx-dependent Ca²⁺ increase up-regulated the formation of the actin coat associated with bacterial vacuoles, suggesting a role for this structure and actin components in vacuolar rupture. Consistently, we found that myosin II and myosin VI were involved in rupture of the *Shigella* vacuole in a Ca²⁺-dependent albeit differential manner. We found that phospho-activated myosin II associates with actin filaments in membrane ruffles distant from the bacterial vacuole. In contrast, local Ca²⁺ increases triggered the recruitment and formation of myosin VI patches contacting the vacuole. Inhibition of myosin VI led to an increased mobility of the bacterial vacuole associated with a delay in vacuolar rupture. The findings suggest that rupture of the *Shigella*-containing vacuole requires Ca²⁺-dependent pulling forces exerted by distal myosin II combined with the tethering of the vacuole in the actin cortex by myosin VI.

Keywords: *Shigella*, vacuole, Calcium, Myosin II, Myosin 6, actin.

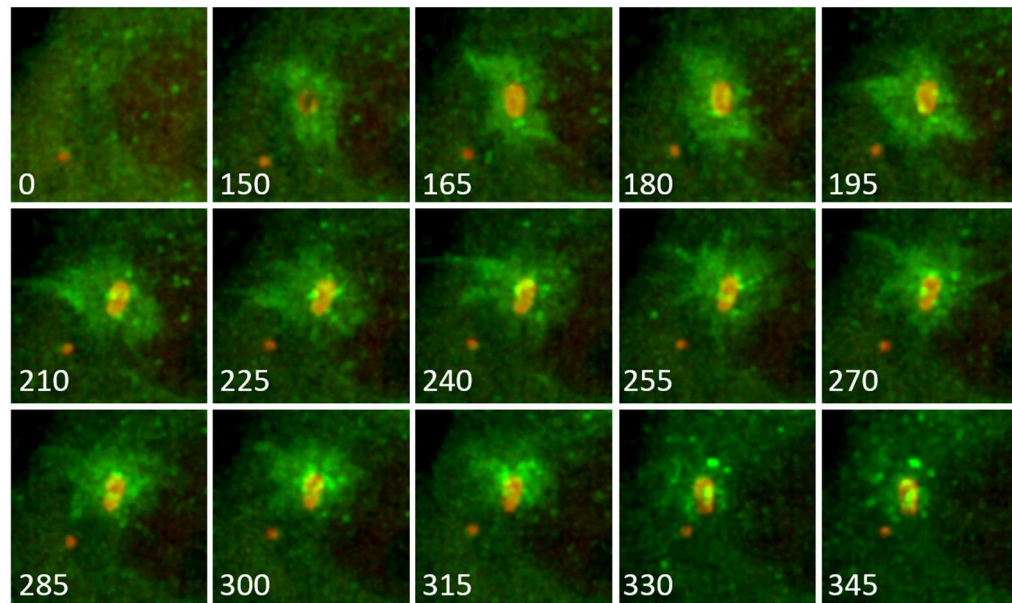


Figure: Time-Lapse fluorescence microscopy analysis of Myosin VI at the *Shigella*_containing vacuole

K-05 **Aptamer-Based Rapid Detection of Biomarkers in Infectious Diseases and Cancer**

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Abstract: Aptamers are short nucleic acid molecules with high affinity and specificity that have become powerful alternatives to antibodies in diagnostic applications. Their stability, ease of synthesis, and tunable chemical modifications make them ideal candidates for rapid and sensitive biosensing platforms. In this study, novel aptamers were developed against two clinically relevant biomarkers: carcinoembryonic antigen (CEA), a key marker for colon cancer, and MPT64, a secreted protein of *Mycobacterium tuberculosis*. Using SELEX combined with next-generation sequencing (NGS), ssDNA aptamers with high specificity and affinity were identified. Their performance was validated using surface plasmon resonance (SPR), enzyme-linked oligonucleotide assay (ELONA), structural predictions, and binding assays in HT-29 colon adenocarcinoma cells for CEA, as well as clinical samples for tuberculosis. To improve sensor performance, different linker and co-adsorbent strategies were explored for aptamer immobilization. Electrochemical impedance spectroscopy (EIS) aptasensors utilizing these strategies achieved detection limits of 81 pM for MPT64 and 2.4 pg/mL (in buffer) and 3.8 pg/mL (in human serum) for CEA. This talk will cover the selection, characterization, and modification of aptamers, demonstrating their integration into EIS-based biosensors and highlighting their potential as low-cost, rapid, and clinically relevant tools for point-of-care diagnostics in cancer and infectious diseases.

K-06 Single-cell analysis using glass nanopipette-based scanning probe microscopy

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Abstract: Dynamic visualization of extracellular chemical concentration gradients around live cells is essential for understanding cellular metabolism, cell–cell communication, and the relationship between chemical gradients and cellular function. Scanning ion conductance microscopy (SICM), which employs nanopipettes with radii under 50 nm, enables non-contact nanoscale topographic imaging, localized chemical delivery, and cytosolic sampling (*Fig.1*). To detect extracellular metabolites, we have integrated nanoscale electrodes¹, electrochemical FET probes², and nanopore sensors³ onto SICM probes, achieving micromolar-level detection of oxygen, pH, catecholamines, and hydrogen peroxide (H₂O₂).

We also developed a hybrid SICM–electrochemical syringe system for localized cytosol collection and subsequent mRNA analysis in living cells^{4,5}. This voltage-controlled syringe allows femtoliter-scale precision and has been used to quantify spatial differences in *Actb* mRNA expression in individual mouse fibroblasts. The same approach has been extended to single-organelle sampling to investigate subcellular metabolite

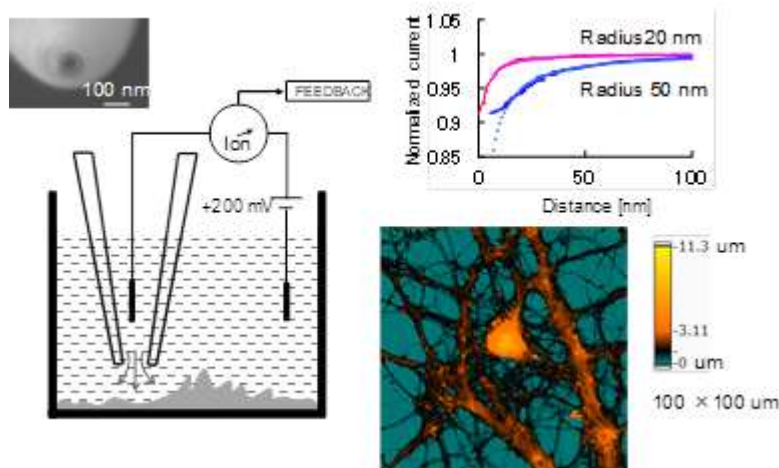


Figure 1 Schematic illustration of SICM and hippocampus neuron topography image.

localization. Furthermore, high-speed SICM has been employed to track dynamic morphological changes by adaptively selecting scan regions based on prior topography, enabling visualization of neurite volume shifts, cargo transport, and growth cone remodeling⁶. In this way, I will introduce various applications of SICM for single-cell analysis that we have developed over the past 20 years.

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2. Zhang, Y. et al. *Acs Nano* 2016, **10** (3), 3214–21.
3. Nashimoto, Y.; Takahashi, Y. et al. *Acs Nano* 2016, **10** (7), 6915–22.
4. Zhang, Y.; Takahashi, Y. et al., *Nat. Commun.*, 2019, 10, 5610.
5. Ida, H.; et al., *Nano Lett.* 2025, **25**(11), 4322–4329
6. Takahashi, Y.; et al., *Anal. Chem.* 2020, 92, 2, 2159–2167

Keywords: nanopipette, live cell imaging

K-07 Micro Elastofluidics: Elasticity and Flexibility for Efficient Microscale Liquid Handling

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Abstract: Although progress has been made in materials development and flexible electronics, microfluidics in wearable and implantable systems remain an almost unexplored area. There are practical and fundamental reasons for the slow progress in this area: (i) current labs on a chip (LOCs) and organs on a chip require bulky lab equipment such as syringe pumps and microscopes to operate, and are not practical for wearable devices; (ii) most wearable systems are continuous-measurement tools that require a different design approach than conventional single-measurement LOCs; (iii) storage of samples in vials and syringes, as well as their continuous delivery using pumps, makes them too bulky and not practical for wearable systems; (iv) the flexible and conformal nature of wearable/implantable systems does not allow for the implementation of established methods in conventional rigid microfluidics; and most importantly, (v) the fundamentals of fluid–structure interactions, and the effect of structural flexibility and elasticity on storage, mixing, separation and delivery of liquids in molecular scale and macroscale, are not understood well enough to enable suitable engineering solutions. This talk presents our recent results in the field of micro elastofluidics, utilising flexibility and elasticity from molecular scale to device scale. Typical examples are enhanced mixing and separation with viscoelastic fluids, liquid storage and handling with liquid beads and tuneable microfluidic devices for separation and handling of biological particles.

K-08 Pushing Optical Tweezers Limits: How Kinesins Walk - It's Not How You Thought!

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Abstract: Simultaneously measuring the nanoscale motion and forces that molecular machines generate provides insights into how they work mechanically to fulfill their cellular function. To study these machines, we developed high-refractive index nanospheres as probes for optical tweezers. With these nanospheres, we have improved the spatiotemporal resolution of optical tweezers and discovered that the motor kinesin takes 4-nanometer sub steps. Further, instead of detaching from their microtubule track under load, motors slid back on it, enabling rapid reengagement in transport. Together with rotation and torque measurements, we have revised how kinesin walks. I will discuss the limits of optical trapping, and the development and application of nanosphere-trapping for biophysical applications. Germanium and silicon nanospheres are promising for many applications in biophysics and nanotechnology. For optical trapping, the nanospheres open a new temporal window by which to uncover hidden dynamics in molecular machines.

K-09 Multiple Mechanisms to Regulate Actin Functions: “Fundamental” versus Lineage-Specific Mechanisms

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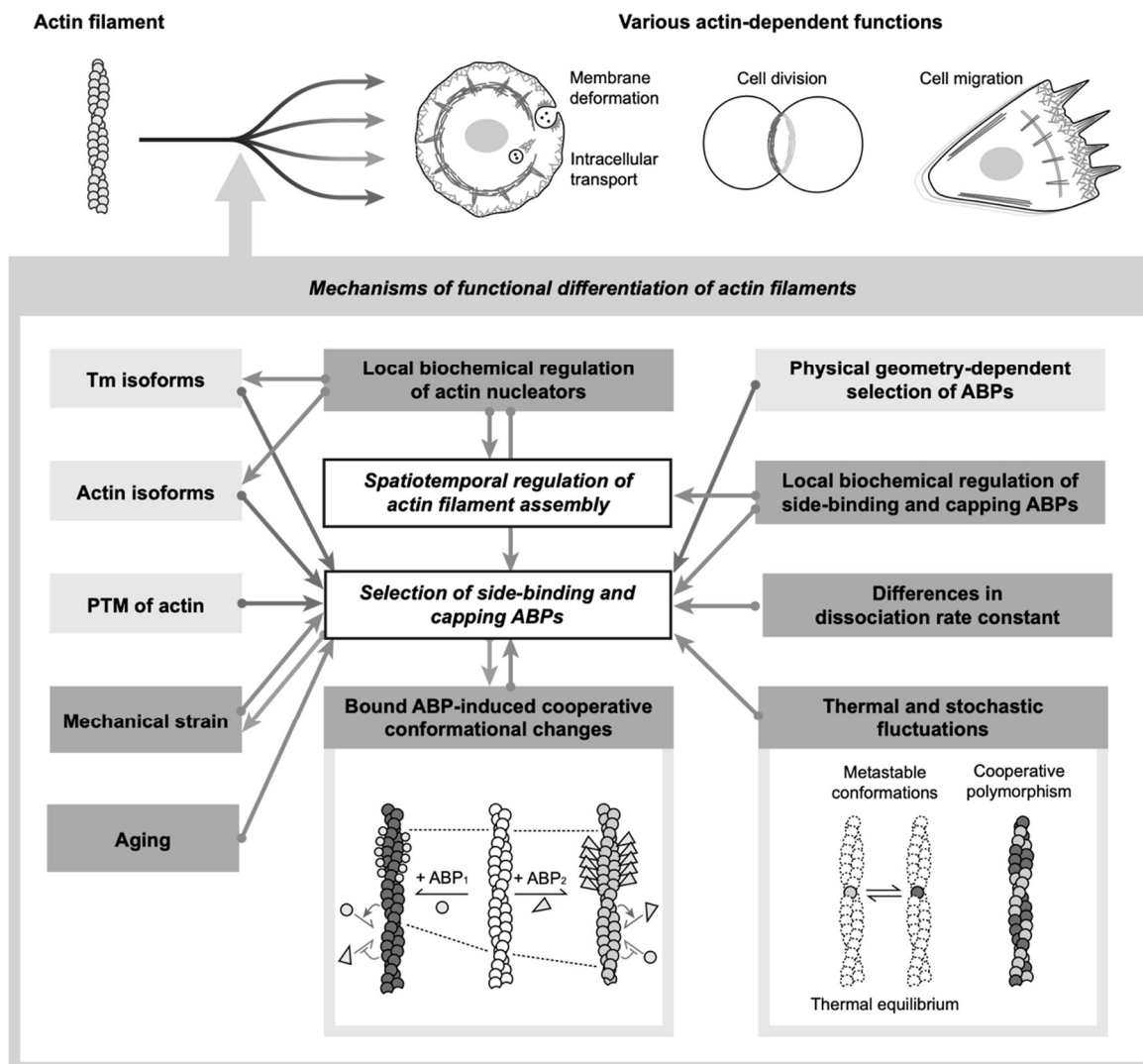
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Abstract: Actin filaments are central to a wide range of cellular functions in eukaryotic cells. Yet, it remains unclear how they simultaneously support distinct functions at different locations within the same cell. Because each function depends on interactions between actin filaments and specific sets of actin-binding proteins (ABPs), understanding how these interactions are regulated is key to resolving this question. Multiple classes of regulatory mechanisms have been proposed and experimentally validated (Figure). These mechanisms differ in both nature and hierarchy: some act downstream of others, revealing layered relationships. Moreover, while certain mechanisms are fundamental and broadly conserved across eukaryotes, others are lineage- or context-specific. We argue that regulation by actin isoforms, tropomyosin (Tm), or post-translational modifications, although important in specific contexts, are not universally essential. Instead, we highlight the fundamental importance of four regulatory principles: (i) biochemical regulation of actin nucleators, (ii) ATP hydrolysis-driven filament aging, (iii) conformational changes of filaments induced by thermal fluctuations and mechanical strain, and (iv) cooperative conformational changes mediated by ABPs. Together, these mechanisms provide a unifying framework for understanding how actin filaments integrate diverse functions within a single cell.

Keywords: *cooperativity; polymorphism; actin-binding protein; aging; biochemical regulation; mechanical strain; nucleator; thermal and stochastic fluctuation*

Figure: Plausible mechanisms of spatiotemporal regulation of actin filament assembly and selection of ABPs. Dark gray shows fundamental mechanisms, whereas light gray shows lineage-specific mechanisms, with arrows showing the regulatory directions. Except for thermal and stochastic



fluctuations, the regulatory processes receive inputs from upstream regulators, which are not shown here. Modified from Uyeda *et al.*, *Biomolecules* 15:279, 2025.

K-10 Unlocking Hidden Local Protein Dynamics with Temporal Resolution Using Geometric Descriptors for Nuclear Receptor in Silico Biophysics

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Abstract: Traditional molecular dynamics (MD) analysis using RMSD and RMSF metrics provides limited insights into protein flexibility, suffering from degeneracy issues and lacking temporal specificity for local dynamics. We introduce GEODES (Geometric Descriptors), a novel computational biophysics framework that enhances MD trajectory analysis through comprehensive 3D geometrical descriptors.

GEODES combines 14 types of protein descriptors across auxiliary, coordinate-derived, and DSSP-derived categories, generating 284 geometrical features that capture comprehensive structural information. The approach integrates Kpax consensus structure determination with DSSP assignments, providing position-independent analysis that eliminates alignment biases while capturing genuine conformational changes with both spatial and temporal resolution.

Applied to vitamin D receptor (VDR) trimeric complexes, GEODES reveals complex-specific behaviors invisible to conventional methods: charge clamp region dynamics crucial for coactivator binding, ligand-binding pocket movements, and quantitative geometric relationships between secondary structure elements. Strong correlations with RMSD clustering (Rand indices 0.923-0.980) validate our approach while uncovering additional conformational information in dynamic protein regions.

The framework's position-invariant descriptors offer powerful applications in computational drug design, providing quantitative measures of binding site adaptability and supporting allosteric modulator development. GEODES represents a paradigm shift in structural biophysics, delivering detailed protein flexibility analysis with broad applications in drug discovery, protein engineering, and biochemical research.

K-11 Design Lipid Nano Carriers Based on Their Interfacial Properties

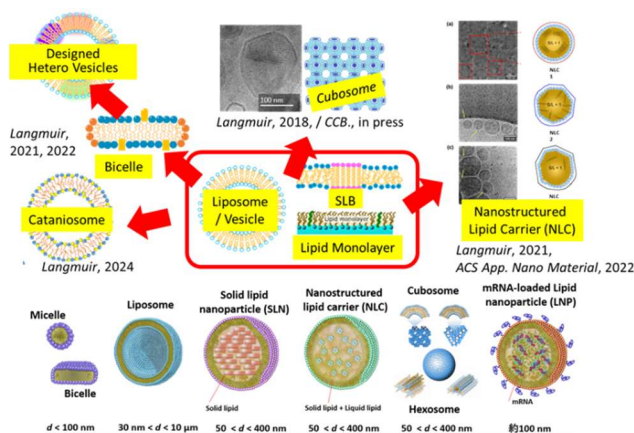
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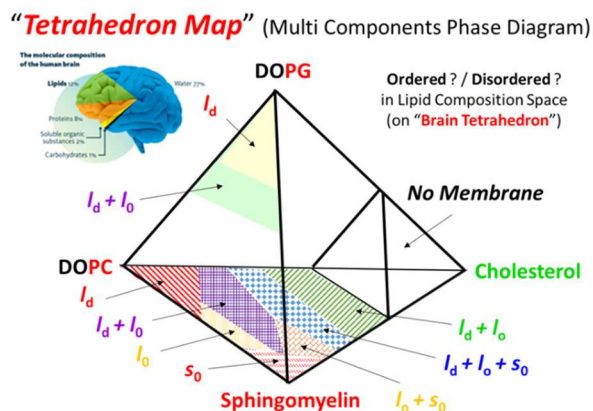
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Abstract: Lipid Nano Carriers (LNC), such as liposome, vesicle, bicelle, cataniosome, nano-structured lipid carrier, cubosome, and so on, can be categorized as lipid vectors for drug delivery systems (DDSs), which are composed of various lipids. In this presentation, a systematic method to characterize the “interface” of various LNCs will be introduced by selecting some case studies. The method includes the (1) conventional physical characterization methods (i.e. DLS, SANS, etc) and (2) (our original) physicochemical ones (i.e. multi-probes fluorescence spectroscopy, time-resolved/decay-associated fluorescence spectroscopy, (surface enhanced) Raman spectroscopy etc). These systematic results can be used to clarify the design space of the LNC composition (i.e. “tetrahedron map”) for the effective DDS.

Keywords: Self-assembly, multi-probes fluorescence spectroscopy, time-resolved /decay associated fluorescence spectroscopy



Design of Self-Assemblies based on Interfacial Properties



Data Space for Interfacial Properties of Self-Assembly

Figure: Target Nano Lipid Carriers and Example of Design Data Space

K-12 Deciphering Ciliary Assembly: Insights Revealed by Cilia Tip Structure

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Abstract: Motile cilia are specialized organelles capable of autonomous movement. Their rhythmic beating generates the forces that propel cells and drive fluid flow. The axonemal skeleton consists of peripheral doublet microtubules and a central pair (CP), with the tip exhibiting a distinctive organization. At this site, microtubules display structural diversity, transitioning between doublets, singlets, and central singlets. The tip is also the hub of ciliary growth, making it a tightly regulated region. Using cryo-EM, cryo-electron tomography, and complementary methods, we analyzed the architecture of the ciliary tip to uncover its regulation and function. In *Tetrahymena thermophila*, we resolved the high-resolution structure of the CP and identified multiple tip-associated proteins with unique binding patterns along the CP microtubules. Notably, the conserved protein SPEF1 binds both microtubule seams, crosslinking the two singlets. In vitro, human SPEF1 also targets the microtubule seam, as revealed by cryo-ET and subtomogram averaging, and stabilizes microtubules in single-molecule dynamics assays. Functional studies in zebrafish showed that SPEF1 knockdown induces heart laterality defects characteristic of primary ciliary dyskinesia. Together, our findings demonstrate that CP-associated proteins stabilize tip microtubules and are critical for preserving axonemal integrity.

K-13 *Drosophila melanogaster* as a rapid, reliable and cost-effective platform for assessing the efficacy of drugs and nanoparticles

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Abstract: *Drosophila melanogaster* is a small fly commonly found near unripe and rotted fruit. It has been widely used for genetic and developmental studies due to its short life cycle, large offspring numbers, and low cost. Here, we show that *Drosophila* neural stem cells or neuroblasts are a fast, and reliable model for assessing the efficacy of newly developed drugs and nanoparticles. In contrast to the time-consuming and expensive in vitro cell viability studies and in vivo animal models, *Drosophila* neuroblasts provide a far more simple, rapid, and cost-effective platform to use. Data from our latest study clearly demonstrates that *Drosophila* neuroblasts are useful in evaluating the efficacy of nanoparticles on cell cytotoxicity, which is comparable to that of cell lines. Live cell imaging, combined with biophysical measurements, is very useful for characterizing the effect of drugs and nanoparticles on the biophysical (mitosis time, cell cycle time, cell shape and size, spindle morphology) and biomechanical (cortical stiffness and intracellular pressure) properties of *Drosophila* neuroblasts in intact brain and in primary culture. This combined approach aims to comprehend the effects and mechanism of action of drugs or nanoparticles when they interact with rapidly proliferating neural stem cells. Data from live cell imaging of intact brains with and without the glial blood-brain barrier will also reveal how drugs and nanoparticles affect the proliferation of rapidly proliferating neural stem cells and their ability to cross the blood-brain barrier. Experiments using these frequently dividing cells would allow us to quickly determine the toxicity and effectiveness of drugs and nanoparticles, as well as enabling higher throughput screening.

K-14 Physics insights in a comprehensive drug design pipeline at the Key Laboratory for Multiscale simulation of complex systems

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Abstract: In this talk, we present recent results from an integrative approach to our traditional computational biomedicine investigations being employed at the Key Laboratory for Multiscale simulation of Complex Systems (KeyLAB), University of Science, Vietnam National University – Hanoi. In collaboration with our Julich and UK collaborators, by combining various computational tools encompassing bioinformatics, data science, machine learning, QM/MM simulation and molecular dynamics, we construct comprehensive biophysical and pharmacological models for screening, design and optimization of biomolecules. Working with in-house experimentalists, in-vitro and in-vivo models are built for cross-checking and further optimization. The KeyLAB is creating a research and implementation pipeline to facilitate traditional biomedicine and biomedical research, quickly transforming initial ideas to practical products, and intellectual properties. Several examples are briefly demonstrated in this talk. The first direction is related to screening and optimization of Vietnam natural compounds toward anti-inflammation disease such as Gout disease or mu-opioid targeting ligand. The second direction is to use our integrative pipeline toward selecting and optimizing aptamer sequence for biosensor detecting neurotoxins or deadly bacteria.

K-15 High-Speed Atomic Force Microscopy and Cryo-EM: Dynamics and Structures of Membrane Proteins

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Abstract: High-speed atomic force microscopy (HS-AFM) is a powerful technique that provides dynamic movies of biomolecules at work. First, I will briefly review our recent developments to break temporal limitations to characterize molecular dynamics by developing HS-AFM line scanning (HS-AFM-LS) and HS-AFM height spectroscopy (HS-AFM-HS) [1], and resolution limitations by developing Localization AFM (LAFM) [2]. Then, I will detail how we used HS-AFM to analyze membrane-embedded TRPV3 at the single-molecule level, and discovered a previously unobserved, transient, and reversible pentameric state of TRPV3, while cryo-EM analysis allowed to resolve the first structure of a pentameric TRP channel [3,4].

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K-16 Learning Protein Motions

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Abstract: Proteins move and deform to ensure their biological functions. Despite significant progress in protein structure prediction, approximating conformational ensembles at physiological conditions remains a fundamental open problem. I will present novel perspectives on this problem and our contributions.

I will first present our recent work on reconstructing protein motions from Atomic Force Microscopy (AFM) images. Indeed, AFM offers a unique opportunity to study the conformational dynamics of proteins in near-physiological conditions at the single-molecule level. However, interpreting the two-dimensional molecular surfaces of multiple molecules measured in AFM experiments as 3D conformational dynamics poses a significant challenge. To address this, we developed AFMfit, a flexible fitting procedure that deforms an input atomic model to match multiple AFM observations [1]. The procedure results in a set of fitted atomic models that form a conformational ensemble describing the AFM experiment. Our method uses a new fast fitting algorithm based on the nonlinear Normal Mode Analysis (NMA) method NOLB to associate each molecule with its conformational state. AFMfit processes conformations of hundreds of AFM images of a single molecule in a few minutes on a single workstation, enabling analysis of larger datasets, including high-speed (HS)-AFM. I will demonstrate the applicability of our method to the membrane-embedded transient receptor potential channel TRPV3 and bound and unbound forms of alpha-actinin [2].

One can also directly target continuous compact representations of protein motions inferred from sparse experimental observations. To do so, we collected protein single-chain statistics from the PDB for a systematic and comprehensive description of protein families conformational variability [3]. Beyond descriptive analysis, we assessed classical dimensionality reduction techniques for sampling unseen states on a representative benchmark. Then, we developed a task-specific loss function enforcing data symmetries, including scaling and permutation operations. Our method PETIMOT (Protein sEquence and sTructure-based Inference of MOTions) leverages transfer learning from pre-trained protein language models through an SE(3)-equivariant graph neural network [4]. When trained and evaluated on the Protein Data Bank, PETIMOT shows superior performance in capturing protein dynamics, particularly large/slow conformational changes, compared to state-of-the-art flow-matching approaches and traditional physics-based models.

Keywords: *AFM, Normal Mode Analysis, Protein Dynamics, Machine Learning*

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K-17 Design of Bimodal Carbon Dots for Dual-Mode MRI and CT Contrast Imaging

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Abstract: The development of safe and efficient multimodal contrast agents remains a key challenge in medical imaging. In this work, carbon dots codoped with iodine and manganese (I,Mn-CDs) were prepared and systematically evaluated as potential bimodal probes for computed tomography (CT) and magnetic resonance imaging (MRI). Incorporation of iodine enabled strong X-ray attenuation, while manganese doping imparted paramagnetic properties beneficial for MRI contrast enhancement. Comparative imaging analysis demonstrated that I,Mn-CDs provide ~19.8% higher CT contrast relative to commercial iopromide solution and ~11.2% stronger MRI signal compared to Gadovist solution under equivalent conditions. In vitro biocompatibility was assessed using normal human dermal fibroblasts (NHDF) and HeLa cells, revealing negligible toxicity across the 0-200 µg/mL concentration range. Obtained results suggest that codoping of carbon dots with iodine and manganese represents an effective strategy for designing next-generation, low-cost, and biocompatible bimodal contrast agents with promising translational potential in diagnostic imaging.

Keywords: Carbon dots, Iodine, Manganese, Bimodal CT and MRI contrast agents, In vitro biocompatibility.

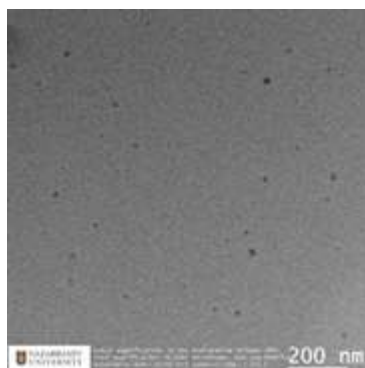


Figure: TEM images of prepared I,Mn-CDs.

INVITED LECTURES

IN-01 Protein engineering for genetically encoded biosensors to visualize cellular metabolism in living tissues

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Abstract: Historically, L-lactate (lactic acid) has been viewed as a waste by-products of glucose metabolism. However, growing evidence suggests that L-lactate is better considered a biological fuel currency and signaling molecule, that can be shuttled over scales and environments ranging from subcellular, to intercellular, to interorgan. To comprehensively explore the emerging roles of L-lactate, methods for monitoring of its concentration in live tissues are of broad utility and high impact. However, there remains a technological gap in high-performance biosensors capable of monitoring L-lactate metabolism in living organisms with high spatiotemporal resolution.

Herein, we present that protein engineering based on directed evolution and rational mutagenesis can enable the engineering of fluorescent protein-based biosensors, designated the LACCO series, for a versatile metabolite L-lactate with high sensitivity, brightness, specificity, and spatiotemporal resolution in living cultured cells and animals. We used these state-of-the-art biosensors to achieve a visualization of the L-lactate dynamics across cellular compartments, revealing an unprecedented L-lactate shuttle in a spatiotemporal manner. We also have resolved their structures and provided insights into their molecular mechanism of lactate-dependent fluorescence response. The latest LACCO series represents a major technological leap towards interrogations of the emerging roles of L-lactate in living cells and tissues.

Keywords: *L-lactate, genetically encoded biosensor, fluorescent protein, protein engineering*

IN-02 Applications of photonic micro and nanostructures in optical biosensors and microbiolasers

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Abstract: The applications of photonic structures for optical biosensors and microbiolasers are introduced in this work. The photonic structures of ZnO nanostructures and ZnO nanostructures decorated with Au nanoparticles (NPs) were implemented for fluorescent non-enzymatic glucose/dopamine sensors. The detection is based on the photoluminescence quenching of the nanostructures exposed to glucose/dopamine. The sensor exhibits a higher sensitivity and a lower limit of detection along with excellent selectivity and a short response time (less than 5s). This is better than previously reported work based on the use of ZnO nanostructures. It is attributed to the high surface-to-volume ratio of the nanostructures, and due to the surface plasmon resonance of the Au NPs. The sensor is applicable to glucose/dopamine detection in human blood serum with high accuracy.

The natural chicken albumen and natural Artemia eggshell-based microbiolaser are also represented. By using a simple but effective fabrication process, rhodamine B-doped chicken albumen microspheres and rhodamine B-doped natural photonic crystal of Artemia eggshells were fabricated. Under optical pulse excitation, these dye-doped microstructures emitted lasing emissions with relatively low thresholds and high Q factors. The lasing mechanisms were investigated and ascribed to whispering gallery mode (WGM) and to random scattering conditions. Interestingly, these microbiolasers could operate in different biological and chemical environments which makes them promising materials for laser-based biological and chemical applications.

IN-03 Enhanced Dengue Virus Detection and Quantification Using a CRISPR-Cas13a-Lipid Droplet Integrated Assay

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Abstract: Dengue has emerged as a growing global health threat, with reported incidence increasing eightfold between 2000 and 2019. In 2023 alone, over 5 million cases were recorded across 80 countries, with outbreaks reported in at least 23. The burden is significant not only in endemic regions such as Vietnam but is also rising in non-endemic areas, including parts of the United States. Dengue is caused by four closely related serotypes of the dengue virus (DENV), allowing individuals to be infected more than once. Subsequent infections are associated with an elevated risk of severe disease due to antibody-dependent enhancement (ADE). Rapid, portable, and highly specific diagnostics are essential for timely clinical management and effective outbreak response. CRISPR-based diagnostic platforms have shown strong potential in this area; however, their sensitivity and specificity rely heavily on the optimal design of guide RNAs (crRNAs). At Ott's Lab, we developed an efficient *silico* pipeline for crRNA selection and established a CRISPR-Cas13a-based diagnostic platform applicable to multiple pathogens. This talk will share recent innovations in applying CRISPR-Cas technology for RNA virus detection, with a focus on experimental data generated from a CRISPR-Cas13a-based assay targeting Dengue virus. Particular attention will be given to the potential of combining this assay with droplet technology to improve detection sensitivity and quantification accuracy.

Keywords: *CRISPR-Cas; crRNA design; Dengue virus (DENV); Dengue serotypes; Diagnostic.*

Acknowledgement: Thi Thu Hoai Nguyen gratefully acknowledges the support from the QBI Scholarship for Women from Developing Nations, awarded by the Quantitative Biosciences Institute (QBI) at UCSF. This support was essential in facilitating her participation in this collaborative research and scientific exchange.

IN-04 Plasma-Assisted Fabrication of Dual Optical Nanomaterials for High-Sensitivity Detection of Aflatoxin B1

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Abstract: Aflatoxin B1 (AFB1), a highly toxic mycotoxin, necessitates the development of sensitive and selective detection techniques to ensure food safety. This work presents a dual-nanotechnology approach using plasma-assisted synthesis methods to fabricate two functional nanomaterials: gold nanoparticles (AuNPs) and carbon quantum dots (CQDs), each tailored for specific optical detection strategies.

Firstly, AuNPs were synthesized via an eco-friendly method utilizing orange peel extract with plasma activation, enabling enhanced nucleation and size uniformity. These spherical AuNPs (~15.9 nm) displayed a strong surface plasmon resonance at 523.5 nm and were employed as surface-enhanced Raman scattering (SERS) substrates. The localized plasmonic effect amplified Raman signals of AFB1, achieving a limit of detection (LOD) of 0.13 ng/mL—superior to conventional HPLC and ELISA methods.

In parallel, CQDs (~4.56 nm), known for their strong fluorescence and biocompatibility, were employed in a Förster Resonance Energy Transfer (FRET) scheme to probe AFB1 interactions. Fluorescence quenching and lifetime reduction confirmed effective FRET, with a Förster radius of 4.81 nm and 46% energy transfer efficiency, resulting in an impressive LOD of 0.439 nM for AFB1. Together, these findings highlight the synergistic potential of plasma-assisted nanomaterial synthesis for developing rapid, sensitive, and environmentally friendly biosensors. The integration of SERS and FRET mechanisms offers a robust platform for comprehensive AFB1 detection in food safety monitoring applications.

IN-05 Development of SERS Substrates Using Nanostructured Semiconductors and Metal Nanoparticles for Pharmaceutical Detection

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Abstract: This study investigates the characterization of Ag/AZO SERS substrates fabricated by different methods for pharmaceutical detection, focusing on how structural, defect-related, surface, optical, and electrical properties of Al-doped ZnO influence sensitivity. The synthesis method significantly affects AZO's surface morphology and electrical behavior: chemical bath deposition yields well-aligned nanorods with a large surface area that enhances light scattering and charge transfer, while DC magnetron sputtering produces rough, highly conductive thin films that boost sensitivity via chemical enhancement. Ag nanoparticles coated on AZO surfaces generate electromagnetic "hot spots," further amplifying the SERS effect. These Ag/AZO substrates effectively enhance the Raman signal of R6G at trace levels. Pharmaceutical compounds were detected using the SERS method based on Ag/AZO substrate performance, in accordance with the ICH guideline Q2(R2) for analytical procedure validation. This demonstrates that SERS is a promising analytical technique, with the Ag/AZO substrate serving as a key component in its application.

Keywords: *SERS, Al-doped zinc oxide, silver nanoparticles, pharmaceutical detection.*

IN-06 Nanoscopic Exploration of the Journey to the Nucleus

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Abstract: Nucleocytoplasmic trafficking is essential for maintaining cellular homeostasis by ensuring precise signaling. Biomolecules travel through selective nanogates known as nuclear pore complexes (NPCs). This process can be hijacked by viruses or become dysregulated in cancers and neurodegenerative diseases. The native structure and dynamics of these biomolecules are critical to understanding disease-related trafficking abnormalities. Conventional structural methods, such as X-ray crystallography and cryo-EM, provide static views and depend on computational modeling to infer dynamics. Fluorescence assays track fluorophore movement but not the molecules themselves. While AFM enables label-free imaging, its low temporal resolution and high tapping forces hinder studies of fragile molecular dynamics. High-speed AFM (HS-AFM), with gentle tapping force (pN level) and fast scanning rates, allows real-time imaging of rapid structural changes without damaging samples. We have investigated several topics related to the trafficking of biomolecules from extracellular regions to the nucleus using HS-AFM. First, we elucidated the conformational dynamics of viral fusion proteins that orchestrate viral entry. Real-time processes, such as the fusogenic transition of hemagglutinin of influenza A virus in an acidic environment, and interactions between the SARS-CoV-2 spike protein and ACE2 or neutralizing antibodies, were recorded using HS-AFM. The SARS-CoV-2 accessory protein ORF6, known to disrupt nucleocytoplasmic trafficking, was also examined nanoscopically with HS-AFM, revealing its potential amyloidogenic properties. In addition, we investigated the structure and dynamics of NPCs isolated from cancer cells and mouse brain tissues to understand nucleocytoplasmic trafficking in both normal physiology and disease states. In summary, we integrate HS-AFM with complementary approaches to address key questions in nucleocytoplasmic trafficking.

Keywords: *nuclear pore complex, nuclear transport, high-speed atomic force microscopy, viral proteins, nanoimaging.*

IN-07 Prebiotic oligosaccharides resembling human milk oligosaccharides: from enzyme production to enzymatic synthesis

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Abstract: The main aim of this study is to find new enzymes that can be promisingly applied to produce mimics of human milk oligosaccharides (HMOs) used for infant food. The substrates of interest are chitin and lactose, which are cheap, abundant in nature and applicable for commercial scale. The aim was hence to obtain oligosaccharides containing both *N*-acetyl- β -D-glucosamine (β -D-GlcNAc) and D-galactose residue, mimicking the core structure of HMOs.

The chitinase gene (*chi*) from *Bacillus licheniformis* DSM13 was expressed intracellularly in *Lactobacillus plantarum* WCFS1, at a level of approximately 5 mg of recombinant protein per litre of cultivation medium. The purified recombinant enzyme shows good thermostability (half lives of stability of 20 and 8.4 days at 37 and 50^o C, respectively), as well as good stability in the pH range of 5–10. The main products of colloidal chitin hydrolysis are various *N*-acetyl-chitooligosaccharides with approximately 1.4 g L⁻¹ produced when using 2.6 g L⁻¹ solubilised chitin.

The *lnbA* gene of *Lactococcus lactis* ssp. *lactis* IL1403 coding for *N*-acetyl- β -D-hexosaminidase was over-expressed in *Escherichia coli* BL21*(DE3) with 89 mg of pure recombinant enzyme obtained per litre of culture. The purified recombinant enzyme showed hydrolytic activity on *N*-acetyl-chitooligosaccharides but not on colloidal chitin or chitosan. Transglycosylation products were not detected, which is in contrast to fungal *N*-acetyl- β -D-hexosaminidases, which have been previously characterised. These data suggest that the role of the *N*-acetyl- β -D-hexosaminidase LnbA may be to degrade chito-oligosaccharides that are produced by the previously described chitinolytic system of *L. lactis*.

β -Galactosidase have been successfully used to produce galactooligosaccharides (GOS) from lactose. Here, the β -galactosidase-encoding genes *lacZ* from *Lactobacillus bulgaricus* DSM20081 in *Lactobacillus plantarum* WCFS1. The recombinant enzyme shows high transgalactosylation activity and was used for the synthesis of GOS, employing lactose at a concentration of 600 mM. The maximum GOS yields were 50% (w/w) of total sugar.

In conclusion, it is promising to use chitinases as well as β -galactosidases to produce *N*-acetyl chito-oligosaccharides from chitin as well as GOS from lactose in large scale. Both of these oligosaccharide products have prebiotic properties and are of interest for various applications in food and feed.

Keywords: Human milk oligosaccharides (HMOs), prebiotics, chitinase, *N*-acetyl- β -D-hexosaminidase, β -Galactosidases

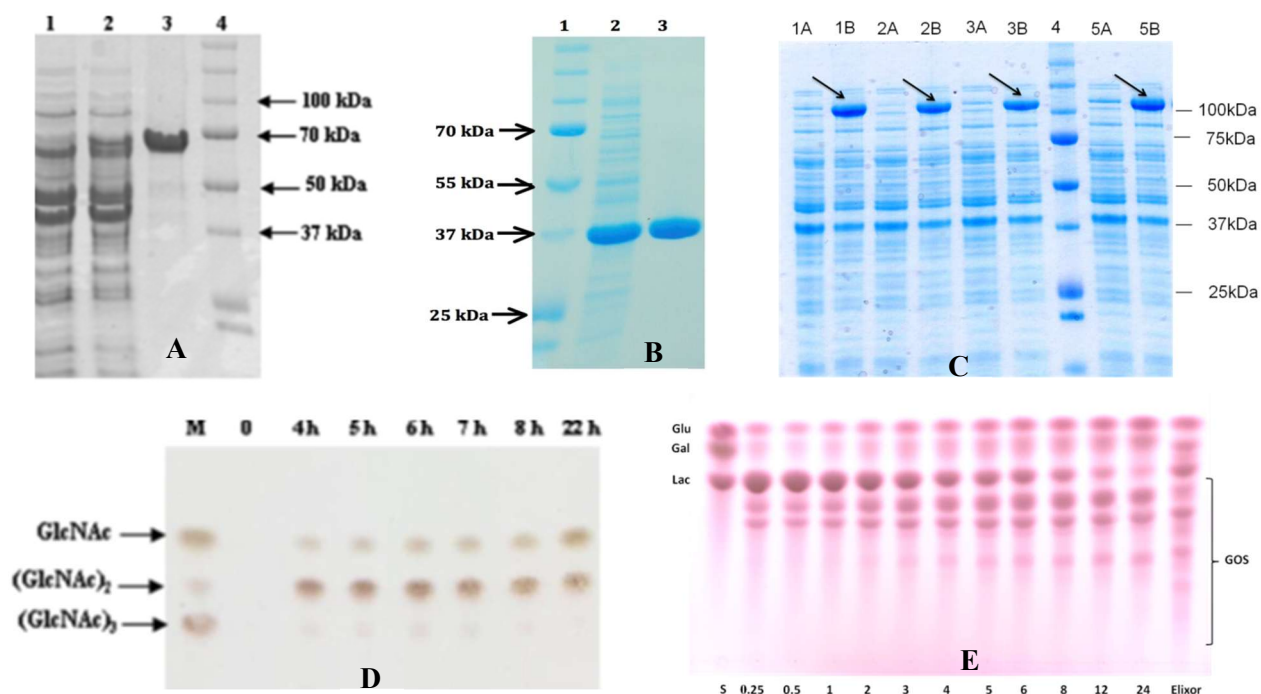


Figure: A, B, C: SDS-PAGE analysis of enzyme expression of genes encoding chitinase, N-acetyl- β -D-hexosaminidase, β -galactosidase, respectively; D, E: Thin layer chromatography analysis of colloidal chitin hydrolysis using recombinant chitinase and GOS production using β -galactosidase respectively.

IN-08 Enhanced delivery of nanomedicines by Au nanoparticles

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Abstract: In our research, we can fabricate nanoparticles (NPs) from pure prodrug molecules, with the size range of 20–100 nm, utilizing the reprecipitation method. This size range is suitable for enhanced permeability and retention (EPR) effect through the abnormally formed tumor vessels with wide fenestrations. By changing the substituents in prodrug molecules, we can partially tune the drug release rate. However, the complexity of the physiological system requires the nanodrugs to overcome various obstacles such as selective cellular uptake or drug resistance, while its surface modification is particularly challenging due to lacking functional groups. Meanwhile, noble metallic nanoparticles (NMNPs) have been extensively studied for drug delivery systems due to their relatively low cytotoxicity and unique plasmonic properties, which can be utilized for cancer detecting/imaging, photothermal therapy (PTT) and photodynamic therapy (PDT). It is known that an extent of charge transfer effect can occur between NMNPs surface and absorbed molecules, which is then utilized in various applications from sensing, bio imaging, catalytic to drug vectorization, etc.

Keywords: *noble metal, drug delivery, cancer therapy*

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IN-09 Bio ceramics and 3D scaffolds for bone tissue engineering

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Abstract: Bone is a dynamic tissue that undergoes continuous remodeling throughout a person's life. It is crucial in providing mechanical support, protecting internal organs, and facilitating body movement. With increasing life expectancy and an aging world population, the incidence of orthopedic-related fractures and pathologies such as osteoporosis, low-back pain, and bone tumors is on the rise. The traditional bone grafts (e.g., autografts and allografts) have been used to restore defective bones. But those treatments demonstrated significant disadvantages: the morbidity associated with a second surgical site, pain from subsequent surgeries, and anatomical complications (for autografts) and potential risk of disease transmission, severe immune response, and limited availability (for allografts).

Bone tissue engineering (BTE) is a promising method for regenerating damaged bones, overcoming the drawbacks of the grafting techniques. The approach involves combining a biodegradable matrix (scaffold), living cells, and biological molecules to produce a construct that promotes the repair and regeneration of targeted tissue. Scaffolds for BTE should possess several properties, such as high porosity, a macroporous network that facilitates cell adhesion, proliferation, and further tissue growth, as well as biodegradability into non-toxic products, and sufficient mechanical strength. To achieve these properties, BTE scaffolds are often designed to mimic the structural and biological functions of a naturally occurring extracellular matrix (ECM) in terms of both chemical composition and physical structure. Bioceramics, including hydroxyapatite (HAp), tricalcium phosphate (TCP), and bioactive glasses, are promising biomaterials for use in bone scaffolds. They are highly biocompatible and possess osteoconductivity properties and a strong affinity to host tissue, supporting mesenchymal cell attachment, differentiation, and proliferation. However, the main drawbacks of those compounds are brittleness, fragility, and difficulty in shaping, which limit their applications alone in fabricating scaffolds for bone repair, especially at load-bearing sites. Polymer/bioceramic composite scaffolds are gaining increasing attention in the field of BTE due to their mechanical stability and biocompatibility. Among such scaffolds, HAp/polymer composites have gained considerable interest due to their composition and structural similarity to natural bone. Chitosan (CS) is a natural polymer derived from chitin, which is found in the exoskeletons of crustaceans. This polysaccharide has a backbone resembling glycosaminoglycans, the primary components of the ECM of bone and cartilage. This similarity makes CS an ideal biomaterial for BTE applications. Moreover, bone is a complex composite that comprises an organic phase (90% type I collagen), minor amounts of lipids and osteogenic factors, and a mineral phase. The mineral phase consists of one or more types of CaP, comprising 65-70% of bone and embedded in a protein matrix. HAp is the most stable CaP in body fluids and is the most similar to the mineral part of bone. The biological HAp found in physiological hard tissues are irregularly rod-like or plate-like crystals of variable lengths and widths (30-45 nm) with a thickness of approximately 5 nm.

In this presentation, we will introduce our recent studies on the development of nano-bioceramics (e.g., HAp, TCP, and SiO₂), which resemble natural bone and are used as an inorganic phase in bone scaffolds and biomimetic scaffolds based on bioceramics/chitosan for bone regeneration.

Keywords: Bioceramics, HAp, Scaffold, Biomimetic, Chitosan, Bone tissue engineering.

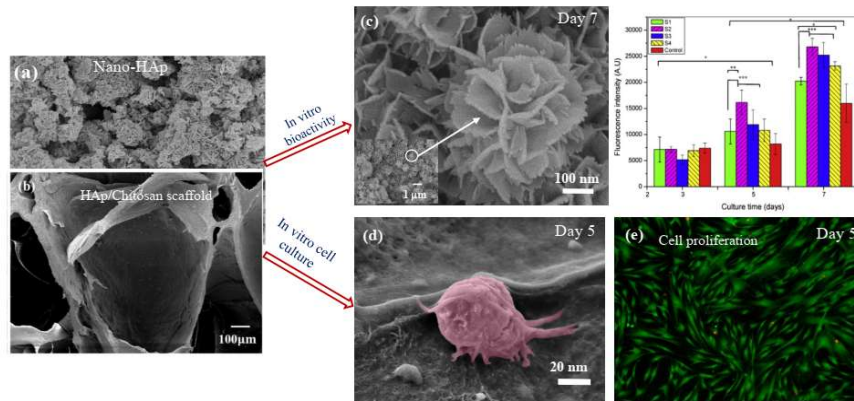


Figure: (a) Nanostructured HAp; (b) Microstructured HAp/CS scaffold; (c) Biomineral layer formed on the surface of the scaffold on day 7; (d, e) Cell adhesion and proliferation on the HAp/CS scaffold on day 5

IN-10 Fabrication of magnetically separable magnetite - graphene hybrid materials with enhanced photocatalytic efficiency for dye degradation

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Abstract: Developing efficient, reusable photocatalysts is crucial for sustainable water treatment. Here, we report a facile plasma electrochemical approach to synthesize magnetically separable magnetite - graphene hybrids with tunable photocatalytic properties. Optimizing the Fe³⁺/Fe²⁺ ratio during synthesis yielded materials with a narrowed band gap, enhanced charge transfer, high surface area, and strong superparamagnetism. After repeated cycles, the optimized hybrid achieved 97.2% methylene blue degradation - 1.5x higher than non-optimized samples - and retained ~ 95% efficiency. These results demonstrate the potential of magnetite–graphene hybrids as high-performance, recyclable photocatalysts for removing organic contaminants from water.

Keywords: Magnetite nanoparticles, graphene nanosheets, plasma electrochemistry, separable photocatalyst, water treatment

IN-11 Electrochemical sensors for trace level detection of heavy metal ions in water by modification of micro electrodes with nano-structured composite layers

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Abstract: The traditional measurement methods such as AAS, ICP-MS, and HPLC can detect the concentration of heavy metals in water in the range of a few parts per billion (ppb). However, these methods are often expensive and time-consuming because they require modern and costly sophisticated equipment, and the analysis process can take a long time. Therefore, electrochemical sensors have been recently developed to detect heavy metals. In this report, the trace level detection of heavy metals like iron and lead in water was introduced using nano-structured layers and nanomaterial blends. The micro metal electrodes were fabricated by micro-fabrication techniques and then working electrodes were modified with nano-structured layers such as Nafion, thermal reduced graphene, blend of polyvinyl alcohol and chitosan. These layers can increase the adsorption capacity towards the heavy metal ions to enhance the sensitivity and selectivity for trace level detection. The electrochemical measurement techniques such as cyclic voltammetry (CV), impedance spectroscopy, anodic stripping voltammetry, linear sweep anodic stripping, square-wave anodic stripping voltammetry (SWASV), square wave voltammetry (SWV), were used. The modified electrodes exhibited a significant enhancement in sensitivity and selectivity for the detection of Pb and Fe. Under optimized conditions, the modified electrode revealed a detection of ppb range with a high correlation coefficient. Moreover, the selectivity study revealed that most common foreign ions did not bring significant interference for Pb and Fe detection.

Keywords: heavy metal ions, electrochemical sensors, nano-structured layers, trace level detection

IN-12 Berberine: latest findings on antibacterial, antiviral and cytotoxic activities

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Abstract: Berberine (BBR), a protoberberine isoquinoline alkaloid derived from various medicinal plants, has gained increasing attention for its diverse pharmacological properties, particularly its antimicrobial potential. Our recent investigations have expanded the understanding of BBR's antibacterial, antiviral, and cytotoxic activities. In antibacterial research, BBR exhibits inhibitory effects against clinically relevant pathogens such as *Escherichia coli*, *Staphylococcus aureus*, and *Salmonella enteritidis*. Innovative formulations with silver and zinc oxide nanoparticles (Ag/BBR and ZnO/BBR complexes) have further enhanced antibacterial efficacy through synergistic physicochemical interactions, enabling bactericidal effects at reduced concentrations and partially overcoming limitations associated with BBR's low solubility and bioavailability. Antiviral studies demonstrate broad-spectrum activity. Notably, *in vitro* assays revealed that BBR markedly inhibited rotavirus replication in MA-104 cells while simultaneously exerting antioxidant and anti-inflammatory effects, thereby mitigating virus-induced cytopathic damage. Cytotoxicity analyses across multiple mammalian cell lines indicate that BBR generally exhibits low to moderate toxicity, with CC50 values ranging from 51 μ M to over 1000 μ M, reflecting cell line-specific sensitivity. Favorable selectivity indices further support its therapeutic potential at pharmacologically relevant concentrations. In conclusion, these findings consolidate evidence that BBR is a promising natural bioactive compound with multifaceted antimicrobial activities. Nanomaterial-based formulations represent a particularly promising avenue to enhance their pharmacological profile, supporting the continued development of BBR-derived agents for the management of infectious diseases.

Keywords: Berberine; antibacterial activity; antiviral activity; cytotoxicity; natural alkaloid

IB-01 Atomic Conformational Dynamics and Actin-Crosslinking Function of Alpha-Actinin Revealed by SimHS-AFMfit

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Abstract: Alpha-actinin is a crucial actin-binding protein involved in cellular functions like muscle contractility, mechanosensation, and cell division. Studying its atomic structure and dynamics is challenging due to protein complexity and imaging limitations. To address this, we developed **SimHS-AFMfit**, integrating high-speed AFM (HS-AFM), AFMfit (a flexible fitting technique), and molecular dynamics (MD) simulations. This approach successfully converted 2D AFM images into 3D atomic conformations, revealing the atomic conformational dynamics of Ca²⁺-bound and unbound alpha-actinin. Using principal component analysis, we classified and quantified protein motions such as twisting and bending. HS-AFM and MD simulations further characterized the fluctuations of rise and axial distance (AD) between adjacent protomers in actin filament crosslinking models, identifying structural features that regulate myosin II and cofilin binding.

These findings enhance our understanding of alpha-actinin's role in actin filament modulation and provide insights for studying more complex protein assemblies, such as contractile rings, stress fibers, focal adhesions, and sarcomeres.

In conclusion, SimHS-AFMfit provides an innovative approach for overcoming the spatial resolution limitations of AFM data [1,2,3]. This method can be further developed, such as by its integration with AI, NMR, cryo-EM, cryo-ET, or in silico AFM, to bridge the spatiotemporal resolution gaps between HS-AFM and the MD simulations and to predict protein dynamics (e.g., deep learning models); this has enabled real-time studies of the atomic conformational dynamics of complex proteins and surpassing the capabilities of individual techniques. Our approach facilitates new possibilities for advancing the understanding of the atomic structural dynamics of complex protein assemblies that mimic cellular machines.

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IB-02 Multiscale AFM Investigation of CRMP2-Microtubule Interactions and Impact on Glioblastoma Cell Mechanics

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Abstract: Collapsin Response Mediator Protein 2 (CRMP2) plays a crucial role in cancer progression, but structural and functional differences between its monomeric and tetrameric forms remain unclear. We present the first High-Speed Atomic Force Microscopy (HS-AFM) study capturing conformational changes of single CRMP2 molecules and their oligomerization dynamics, as well as their impact on microtubule organization. Using conventional AFM, glioblastoma cells expressing CRMP2 monomers or tetramers were analyzed for morphological and mechanical changes, with the monomeric form inducing more pronounced alterations in cell surface topography and stiffness. Nanomechanical characterization by HS-AFM further revealed distinct differences in how monomers and tetramers organize microtubules. These findings demonstrate that CRMP2 oligomerization significantly influences its function in glioblastoma cells, potentially affecting migration and invasion. This study underscores the value of advanced AFM techniques for linking protein structure to cellular function and highlights CRMP2's quaternary structure as a potential therapeutic target in cancer. Together, the multiscale AFM approach provides comprehensive insights, ranging from molecular conformational dynamics to cellular mechanics, thereby enabling a deeper understanding of protein function in complex biological contexts.

Keywords: *Collapsin Response Mediator Protein, Microtubules, Cell Mechanics, Atomic Force Microscopy, Glioblastoma*

IB-03 How biomechanics shapes plant organs

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Abstract: Plants produce organs of various shapes and sizes. While genetic regulation of organogenesis in plants has been extensively studied, the role of biomechanics just started to gain attention in recent years. Unlike animal cells, plant cells are enclosed in a stiff yet extensible cell wall (CW). The growth of a plant cell is the result of the interaction between the turgor pressure caused by water accumulation and the physical properties of the CW (e.g. stiffness) which resists this pressure. CW properties therefore determine how a cell or a tissue growth, and eventually control the shape and size of the final organ. To illustrate this, I will take an example from the formation of the sepal on the flower of the plant *Arabidopsis thaliana*. In this and many other species, sepals are the outermost flower organ which plays important roles, including protection. They fulfill this function by curving inwards to form a closed structure in which reproductive organs are protected. I will show that this inward curving of the sepal is caused by differential growth between two regions – the tip and the body – of the sepal, which forces the sepal to grow more in 3D, i.e. curving. This hypothesis is validated by analog and computer modeling, as well as in planta experiments. I will further show that to maintain this inward curving, the relative growth between the inner side and the outer side of the sepal also needs to be regulated. When the inner side grows faster than the outer side, the sepals bend outwards and the flower is opened prematurely. Overall, these examples illustrate how biomechanics of differential growth controls the shape of plant organs.

Keywords: *biomechanics, organogenesis, plants, cell wall, stiffness, differential growth*

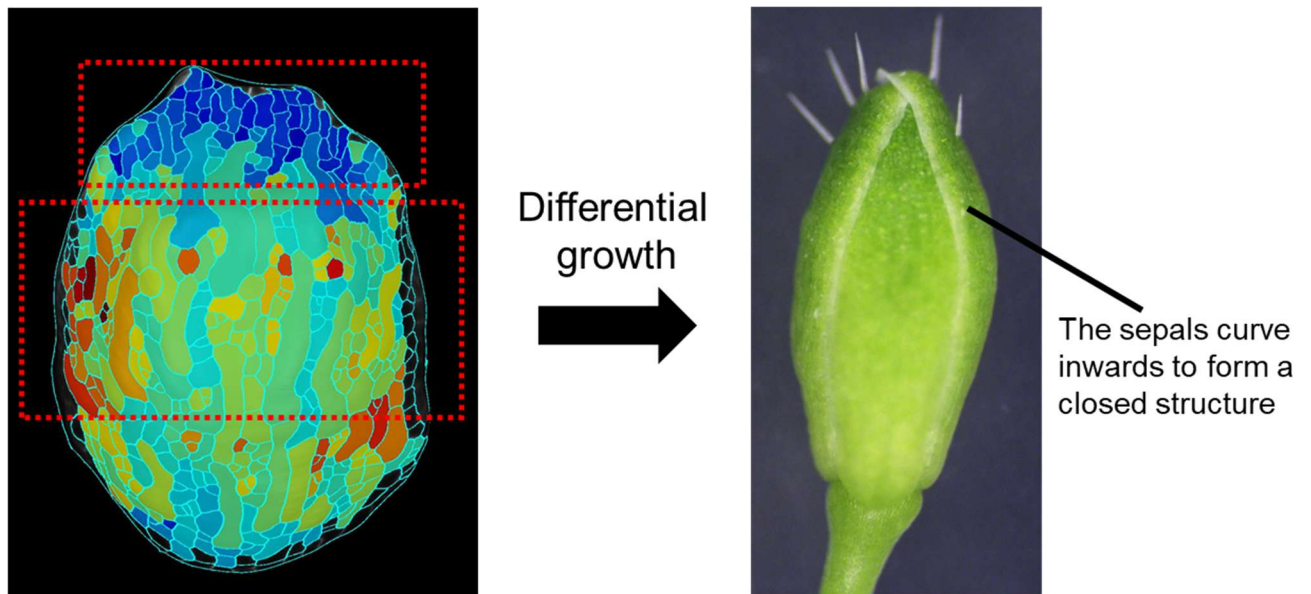


Figure: The sepal of the Arabidopsis plant is curved inwards due to the differential growth between the sepal tip and sepal body (red boxes).

IB-04 Translation dynamics and impact of ribosome structure at the nanoscale

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Abstract: The ribosome is a molecular machine made of RNA and protein complexes, that mediates the translation of mRNA into protein. While ribosomes were traditionally thought to be homogeneous, recent work has discovered that their composition is highly heterogeneous, with important consequences on the regulation of translation. By using a variety of mathematical and computational approaches, we have recently quantified the extent of such heterogeneity and its impact across multiple scales, with a specific focus on the ribosome exit tunnel, a narrow cavity of the ribosome that contains the nascent protein. To facilitate the data processing of all the ribosome 3D structures available from cryogenic electron microscopy (cryo-EM), we developed an online database that provides organized and curated access to ribosome structures with specialized visualization tools. This notably allowed us to compare the geometry of the ribosome exit tunnel across species, and detect new prokaryotic-like ribosome exit tunnels within eukaryotic kingdoms. In addition, we jointly developed coarse grained methods to represent the tunnel geometry and perform simulations of the elongation and escape of the nascent chain during translation, allowing us to investigate various biological processes associated with translation. If time allows, I'll finally mention how this work relates to our more general goal of developing metrics for 3D shapes and Deep learning methods for cryo-EM, with various applications for analyzing biological data.

Keywords: *Protein translation, Ribosome, Ribosome heterogeneity, Molecular Dynamics, Bioinformatics, Cryo-EM, Coarse-grain model, biological shape analysis*

IB-05 Shear-induced fibronectin fibrillogenesis: Differential mechanisms under high and low shear stress conditions

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Abstract: The extracellular matrix (ECM) is highly dynamic and responsive to mechanical cues, particularly shear stress within the vascular microenvironment. In this talk, I will present our recent work demonstrating that fibronectin (FN) fibrillogenesis can be initiated by shear stress in the absence of cells and that both high (2000–5000 s⁻¹) and low (50 s⁻¹) shear regimes drive fibril formation through distinct molecular pathways. Using a microfluidic platform, we replicated physiologically relevant flow conditions to observe FN *remodeling in vitro*. Our results revealed that high shear promotes rapid formation of thick, interconnected fibrils through strong domain-domain interactions, while low shear induces slower assembly via weaker intermolecular binding. Molecular docking identified critical interdomain interfaces between FNI_{1–5} and FNIII_{1–3}, stabilized by specific salt bridges and hydrogen bonds. These findings provide mechanistic insight into shear-regulated ECM assembly and offer a foundation for integrating mechanobiology into vascular omics research.

IB-06 Thermogenetic toolkit for controlling cellular function

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Abstract: The ability to control the activity of target proteins in live cells enables the manipulation of cellular processes. Various approaches have been developed to achieve precise protein regulation. Chemogenetics uses chemical reagents to enable protein-protein interactions. However, achieving single-cell control with high spatial and temporal precision remains challenging. Optogenetics, which uses light-sensitive proteins, offers precise spatiotemporal regulation of ion channels or intracellular proteins through visible light. Despite its advantages, visible light has limited tissue penetration and can unintentionally activate endogenous photoreceptors. In contrast, thermogenetics uses temperature-sensitive proteins to modulate cellular functions through controlled thermal stimuli. This approach enables deeper tissue penetration and offers a practical alternative to optogenetics. Here, we introduce a thermogenetic toolkit for regulating programmed cell death through heat-activated human caspase 8 (CASP8) using thermal-responsive elastin-like polypeptides (ELPs). ELPs exhibit a temperature-dependent phase transition from a soluble state to a coacervate state. We engineered a fusion protein (ELP-CASP8) in which the ELP motif underwent coacervation above 35 °C, thereby increasing the local concentration of CASP8 to promote dimerization-induced activation and apoptosis in HEK293T cells, as confirmed by apoptosis and cytotoxicity assays. To monitor CASP8 activation, we developed a fluorescent CASP8 indicator and validated its functionality in HEK293T cells. We further employed localized optical heating using a 1470 nm laser in combination with fluorescence lifetime-based thermometry to achieve single-cell activation of CASP8 with precise and controlled temperature increments.

Keywords: *thermogenetics, elastin-like polypeptides, caspase8*

IB-07 Large Scale Simulations of Highly Flexible and Dynamical Proteins in Cellular Signaling

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Abstract: Many proteins have well-defined tertiary structures and disordered tails that contribute differently to their functions. A well-defined part can be predicted by AI/ML algorithms, which, however, may fail to gain insights into the roles of unstructured loops between key domains or a disordered tail. In this talk, I will show how large-scale simulations via leadership supercomputers at Oak Ridge National Laboratory (ORNL) help to reveal the roles of two highly flexible and dynamical proteins, which play essential roles in cellular signaling mechanisms. One protein, which is called C-Raf kinase contributing Rapidly Accelerated Fibrosarcoma in aberrant Ras-Raf-MEK-ERK signaling pathways, has three distinct domains for differentiable roles; however, the interdomain interactions and dynamics remain unclear. The other protein, called Arrestin, uses its relatively long but foldable C-tail to inhibit its activation in various signaling pathways that include a large family of G-proteins (GPCRs). These two exemplary cases may suggest important diversely complicated dynamics of proteins that remain to be discovered by large scale simulations and AI-based models, which can be enabled by large computing resources at ORNL allocated via Director's Discretionary and INCITE programs to all competitive proposals around the globe.

Keywords: *Simulations, Protein, Cellular Signaling, Artificial Intelligence/Machine Learning*

IB-08 M cells or not to M cells: an update

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Abstract: Developing oral vaccines via rerouting antigens to immune cells in intestinal tracts has caught much attention recently. As an antigen sentinel and capture port in the gut, M cells are targeted to increase antigen reception, thereby enhancing mucosal immune response. Many studies showed that 60 kDa heat shock protein (Hsp60) from *Brucella abortus* interacts with PrPC exclusively expressed on the M cells surfaces. However, using the whole Hsp60 as an antigen-fused navigator is not an ideal and feasible approach. In this study, a Hsp60 derived, M cell targeting peptide termedly PEP was in silico predicted, genetically synthesized, and in vivo evaluated for mucosal and systemic immune response enhancement. The recombinant plasmid pET22b-pep1-gfp was constructed. Protein PEP1-GFP was induced with IPTG and confirmed by SDS-PAGE and Western Blot. Recombinant protein was purified by metal ion affinity chromatography. Interoperability of PEP1-GFP with PrPC was measured by Silicon Nanowire Field effect transistor (SiNW FET). Finally, the ability of supporting in vivo immune response of PEP1-GFP was evaluated through oral administration on mice. Antibody titer was detected in mice stool and serum. Results showed PEP1-GFP was expressed mainly in soluble fraction and purified by affinity chromatography metal ions with purity above 90%. Then, SiNW-FET results showed the interaction between PEP1-GFP and GST PrPC via changed amperage value on nanofibers compared to GST. Finally, ELISA results showed that the mucosal and systemic immune responses were initiated in the mice given PEP1-GFP protein, and these responses outperformed them in the mice given GFP. These data indicated that PEP1 was able to guide antigen to M cells, enhance mucosal and systemic immune responses.

Keywords: Hsp60, M cells, molecular docking, molecular dynamics, mucosal vaccine

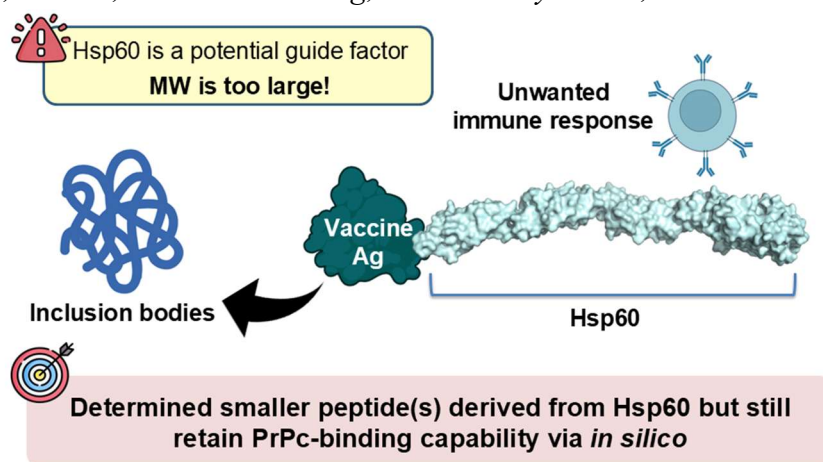


Figure: Hsp60-derived peptide(s) from *in silico* prediction

IB-09 Decoding Gene Regulation Mechanisms and Target Cancer-Causing Proteins

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Abstract: Cell development is orchestrated by a complex interplay among transcription factors, cis-regulatory DNA elements, noncoding RNAs, and three-dimensional genome architecture. Dysregulation of these processes can lead to cancer. Through integrative, genome-wide analyses of gene expression, chromatin accessibility, DNA methylation, histone modifications, and chromatin topology, we identified cell type-specific enhancers regulated by the master transcription factor PU.1. These enhancers—characterized by open chromatin, hypomethylation, and active histone marks—activate lineage-specific genes and are spatially organized within CTCF-defined chromatin domains. Beyond protein-coding genes, PU.1 also regulates enhancer-derived noncoding RNAs, including the enhancer RNA LOUP, which originates from a conserved PU.1-bound enhancer cluster. Functional studies revealed a previously unrecognized transcription factor–noncoding RNA circuit that is critical for lineage commitment and immune function. Leveraging these mechanistic insights for therapeutic discovery, we developed TLigBind, a high-performance computing-based molecular docking pipeline and web application for identifying small molecules targeting oncogenic proteins such as the CBFB::MYH11 fusion and mutant KRAS. Together, our work aims to elucidate the regulatory logic of normal cell development, reveals how its disruption drives tumorigenesis, and provides computational tools for rational, structure-based oncogene targeting.

IB-10 Docking and Molecular Dynamics Study of Silk Fibroin Interactions with Carbon Nanotube

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Abstract: Silk possesses superior mechanical properties, high biocompatibility, and elasticity, along with inherent fibers and enduring strength, making it an ideal material for a wide range of applications. Recent studies have indicated that the structure and functionality of fibroin can be enhanced by incorporating nanomaterials such as graphene or Carbon Nanotubes (CNTs). This work builds upon prior research by utilizing Molecular Dynamics (MD) simulations to investigate the interaction between silk and a CNT in an acidic environment similar to that of a silkworm's stomach. The objective of this work is to use docking techniques to predict the active residues on silk that interact with CNTs, and to subsequently test these predictions through MD simulations involving a single CNT. By confirming the expected active binding sites, this study aims to explore fundamental processes such as π -based interactions and hydrophobic forces that facilitate the preferential accumulation of CNTs at these specific locations. Ultimately, this research seeks to provide molecular-level insights that could lead to the development of advanced composite materials with enhanced mechanical and electrical properties, thus presenting exciting applications in biomedical engineering, advanced textiles, and flexible electronics.

Keywords: *silk fibroin, Carbon Nanotubes (CNTs), Molecular Dynamics (MD) simulations, acidic environment*

IB-11 Cancer detection and classification utilizing polarized/medical images and artificial intelligence (AI) models

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Abstract: Detecting cancer in the early stage plays a crucial role in reducing mortality rates. Although conventional clinical tests are generally reliable, they often lack accessibility during early stages - particularly when biopsies are invasive and require specialized personnel and facilities. In recent years, polarimetric imaging systems have emerged as promising tools in biomedical applications, including tissue morphology characterization, cancer staging, and detection. Besides, machine learning provides a powerful tool for performing the objective and precise diagnosis of cancer through its use of statistics, probabilistic algorithms, and massive computational power.

This study introduces a novel framework for cancer detection and classification by integrating polarimetric imaging - specifically Mueller matrix image analysis - with machine learning techniques. The approach leverages the optical properties encoded in the 16 Mueller matrix elements, alongside medical imaging data, to differentiate between healthy and malignant tissues. Targeted cancer types include skin, breast, liver, blood, and colorectal cancers, where multiple optical effects may coexist. Using in vitro measurements from mouse models, we perform statistical analyses on both Mueller matrix and conventional medical images to extract discriminative features. These features are then used to train machine learning models capable of automated tissue classification.

The results demonstrate that the proposed framework offers significant potential for developing AI-driven diagnostic tools, enabling non-invasive, accurate, and efficient cancer screening.

Keywords: *Polarimetric imaging, cancer detection, Mueller matrix, machine learning, biomedical optics, tissue classification.*

IB-12 Structures and Dynamics of Large RNA Molecules Explored with Coarse-Grained Simulations

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Abstract: RNA molecules are actively involved in various intracellular regulatory processes in which molecular tertiary structures play an essential role. They also hold significant potential for use as a therapeutic molecule, yet the lack of detailed structural information complicates rational and optimal formulation. Experimental techniques, such as cryo-electron microscopy and chemical probing, have demonstrated that messenger RNAs (mRNAs) can form heterogeneous secondary structures, often with transient tertiary interactions. However, fully identifying tertiary structures and higher-order RNA-RNA interactions remains challenging.

Molecular simulation presents an attractive method for acquiring structural information at a resolution unattainable through experimental means. To simulate large RNA structures within the context of cellular function and therapeutics, we have developed a novel simulation model of RNA at nucleotide resolution. Building on a previous model designed for the phase separation of repeat RNA sequences, we have generalized the model to accommodate arbitrary RNA sequences. The model was validated by comparing simulation results with experimental data, such as melting profiles, chemical probing, force response by optical tweezers, and scattering data of longer RNAs.

In this talk, I will present our recent efforts to simulate heterogeneous structures of long RNA strands, such as mRNA and viral genome RNA. As an example, guided by experimental data, we used our simulation model to construct three-dimensional structures of a long self-amplifying mRNA (saRNA; 11,551 nts) at different salt concentrations. This structural information could provide insights into how we might efficiently formulate these therapeutic RNAs with cationic lipids or polymers.

Keywords: *RNA folding, Coarse-grained model, Molecular simulations*

ORAL PRESENTATION

O-01 Application of Atomic Force Microscopy in Materials Science and Cosmetics: Exploring the nanostructural, mechanical and chemical properties

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Abstract: Atomic Force Microscopy (AFM) is an essential tool for analyzing the nanoscale mechanical properties of various materials. It provides key insights into elasticity, adhesion, and hardness, which are crucial for understanding material behavior under different conditions.

In the cosmetics industry, AFM has been employed to study the mechanical properties of products such as foundation, lipstick, human skin, and hair fibers. A deeper understanding of these properties and their nanostructures facilitates the development of natural, health-conscious, eco-friendly cosmetics and more effective formulations.

In biomedicine, AFM has been utilized to study the viscoelastic properties of hydrogels used in tissue engineering. By tailoring the elasticity and viscosity of hydrogels to match the kPa-range modulus of cells, AFM contributes to the design of more effective scaffolds for cell culture.

Similarly, in maritime engineering, AFM aids in assessing the adhesive properties of organic materials like barnacle cement. This research paves the way for developing potent underwater bioadhesives that can also be applied in tissue engineering to protect wounds from external factors and microorganisms, accelerating healing, enhancing treatment efficacy, reducing recovery times, and lowering the risk of infection.

Beyond mechanical analysis, nanoscale chemical mapping is made possible through advanced techniques such as AFM-IR, which combines AFM with infrared spectroscopy. Using techniques like Resonance Enhanced Force Volume (REFV) AFM-IR, one can measure molecular vibrations and obtain distinct infrared spectra at the nanoscale. This approach allows the acquisition of IR absorption spectra and images with spatial resolutions of 50–100 nanometers, making it a powerful tool for studying complex and heterogeneous materials, including block copolymers, cosmetics, and biomaterials.

AFM is a cutting-edge technology with immense potential for investigating nanostructures and their mechanical and chemical properties, establishing itself as a valuable tool in materials science, biomedicine, cosmetics, and beyond.

Keywords: *Atomic Force Microscopy, AFM, AFM-IR, mechanical properties, chemical mapping,*

O-02 The Role of Entropy Production and Spectral Gaps in Giant Diffusion

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Abstract: A fascinating phenomenon in systems driven far from equilibrium is giant diffusion—the dramatic enhancement of diffusive motion observed in molecular machines like the F1-ATPase motor. While the Thermodynamic Uncertainty Relation (TUR) establishes a fundamental lower bound on fluctuations based on entropy production, it cannot explain the exceptionally large fluctuations that give rise to this effect.

We derive a general inverse Thermodynamic Uncertainty Relation (iTUR) that establishes an upper bound on current fluctuations, applicable to both continuous Langevin systems and discrete Markov jump processes. Our relation reveals that the maximal fluctuation is governed by an interplay between the entropy production rate and the system's relaxation timescale, quantified by the spectral gap of a symmetrized operator. A key consequence is that large fluctuations can only emerge from either a high entropy production rate or a small spectral gap (i.e., slow relaxation).

Applying the iTUR to systems exhibiting giant diffusion, we demonstrate that this phenomenon originates from a precise combination of these two factors. The system is driven far from equilibrium by high entropy production, while a simultaneously small spectral gap allows the resulting large fluctuations to persist over long timescales. Our work therefore provides a unifying framework, directly connecting the macroscopic observation of giant diffusion to the fundamental thermodynamic and kinetic properties of the underlying system.

Keywords: *Molecular Motors, Nonequilibrium Steady States, Current Fluctuation.*

O-03 Preparation, Characterization, and Evaluation of Silver Nanoparticles from *Allium cepa* L. Peel Extract

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Abstract:

Background: The limitations of herbal medicines, particularly their poor solubility, bioavailability, and stability, have hindered their effectiveness despite widespread traditional use. Nano drug delivery systems (NDDS), including phytophospholipid complexes and silver nanoparticles (AgNPs), offer a novel approach to enhance the therapeutic potential of plant-derived compounds. *Allium cepa* L. (onion), rich in bioactive compounds such as quercetin and organosulfur compounds, possesses proven antioxidant, antimicrobial, and anti-inflammatory properties. However, challenges in effective delivery limit its clinical applications. This study addresses these challenges through the green synthesis of AgNPs using *Allium cepa* L. peel extract, aiming to improve stability, bioavailability, and therapeutic efficacy.

Aim: To formulate, characterize, and evaluate a herbal nanoextract containing *Allium cepa* L. extract, with a focus on synthesizing silver nanoparticles (AgNPs) and assessing their physicochemical properties and antibacterial activity.

Materials and Methods: Ethyl acetate extraction was used to isolate phytoconstituents from *Allium cepa* L. peels. Preliminary phytochemical screening was conducted to identify active secondary metabolites. Green synthesis of AgNPs was achieved by reacting the extract with silver nitrate solution, indicated by a visible color change. Nanoparticles were characterized using:

- **UV-Vis Spectroscopy:** To determine surface plasmon resonance.
- **Fourier Transform Infrared Spectroscopy (FTIR):** For identifying functional groups involved in nanoparticle formation.
- **X-ray Diffraction (XRD):** To confirm crystalline structure.
- **Field Emission Scanning Electron Microscopy (FE-SEM):** For morphological and size analysis.

The antibacterial activity of the synthesized AgNPs was evaluated using the disc diffusion method against pathogens including *Staphylococcus aureus*, *Enterococcus*, *Escherichia coli*, *Salmonella typhi*, *Pseudomonas spp.*, *Klebsiella pneumoniae*, *Bacillus thuringiensis*, and *Candida albicans*.

Results: Phytochemical screening confirmed the presence of flavonoids, proteins, carbohydrates, and amino acids in the *Allium cepa* L. extract. The color change from yellow to brown indicated the successful synthesis of AgNPs. UV-Vis analysis showed a distinct peak at 445 nm, confirming nanoparticle formation. FTIR spectra revealed functional groups such as hydroxyl, carboxyl, and amine, suggesting their role in reducing and stabilizing AgNPs. XRD patterns showed characteristic

crystalline peaks at 2θ values of 35.45° , 44.32° , and 65.25° , confirming the nanocrystalline nature of the particles. FE-SEM images revealed spherical, uniformly distributed nanoparticles with a size in the nano range (~ 500 nm).

The AgNPs demonstrated significant antibacterial activity, particularly against Gram-positive bacteria. The zones of inhibition observed in the disc diffusion assay confirmed their potent antimicrobial efficacy, supporting their use in combating pathogenic microorganisms.

Conclusion: This study successfully developed and characterized a green-synthesized herbal extract using *Allium cepa* L. extract. The AgNPs exhibited promising physicochemical stability and broad-spectrum antibacterial activity. These findings highlight the potential of *Allium cepa*-based nanomedicine as a sustainable and effective therapeutic agent. Future directions include *in vivo* pharmacokinetic studies, cytotoxicity evaluations, and formulation of topical or oral dosage forms for clinical applications in antimicrobial therapy.

Keywords: AgNPs, *Allium cepa* L., FE-SEM, Herbal nano extract

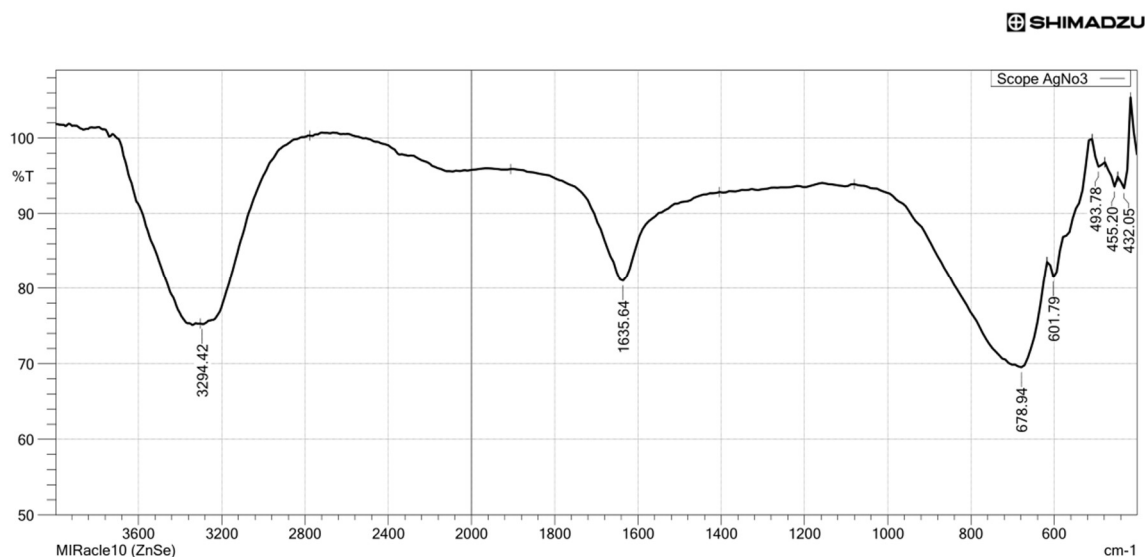


Fig.1. FTIR analysis of AgNPs

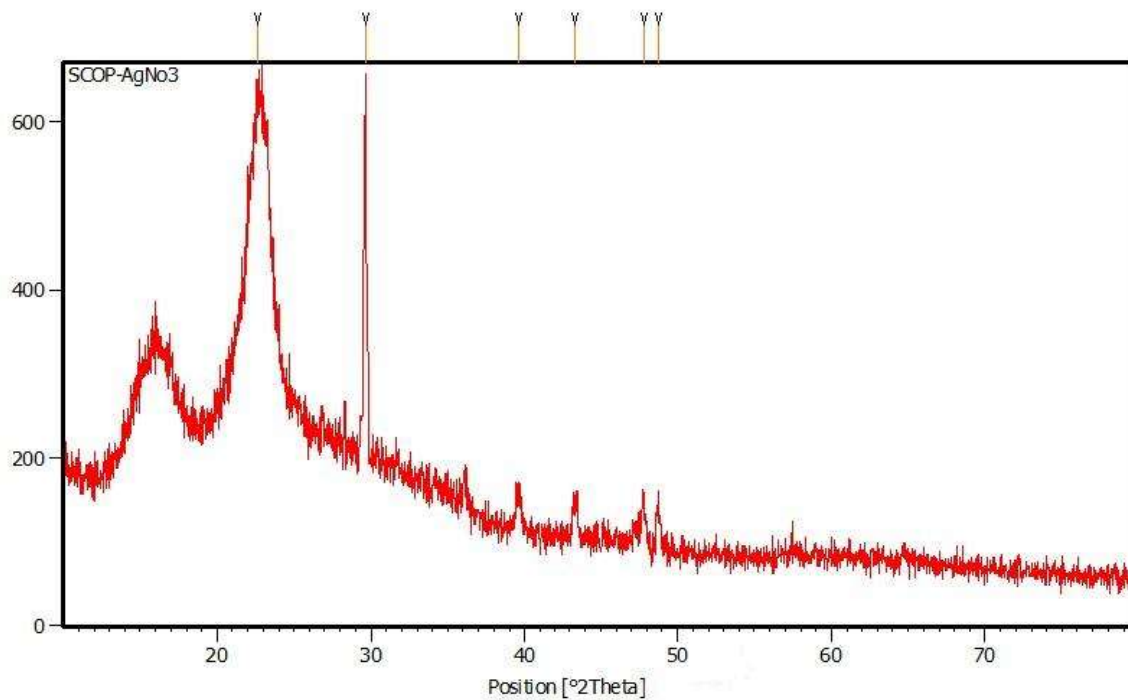


Fig. 2. XRD analysis of AgNPs

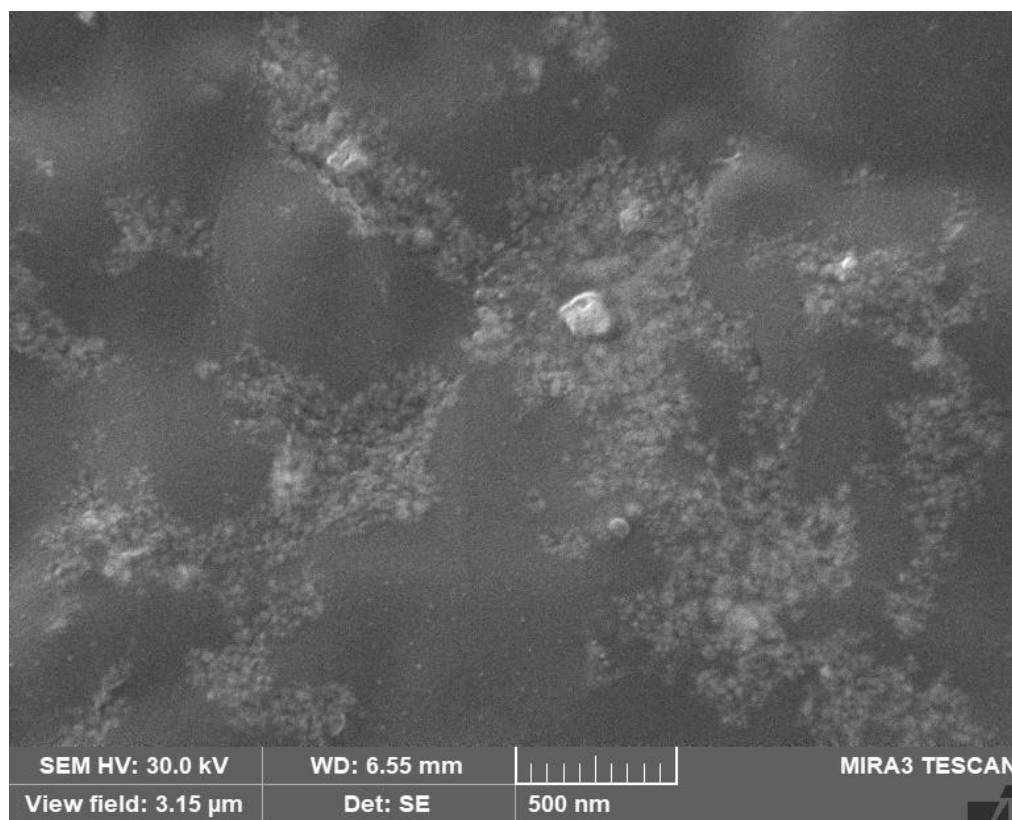


Fig.3. FE-SEM images of AgNPs

O-04 Advanced biosynthesis to boost the production of natural antibiotics for antimicrobial applications

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Abstract: The emergence of biofilm-associated infections and antimicrobial resistance requires innovative strategies that go beyond traditional medicines. In this study, a multi-modal method including co-culture analysis, electrochemical stimulation, and nanoparticle-based enhancement is used to examine the antibacterial efficacy of *Lactobacillus plantarum* against *Staphylococcus aureus*.

Three distinct *Lactobacillus* species were co-cultured with *S. aureus* in a compound medium (CM) that was designed to mimic competitive polymicrobial environments and satisfy both organisms' metabolic needs. The most potent inhibitory effect was shown by *L. plantarum*, which dramatically reduced *S. aureus* planktonic growth and biofilm development in both aerobic and anaerobic settings. In anaerobic, unadjusted pH conditions, cell-free supernatants (CFSs) from *L. plantarum* demonstrated strong antimicrobial activity, with zone of inhibition (ZOI) values as high as 11.5 ± 1.5 mm. Activity was significantly decreased with pH neutralization, demonstrating the significant contribution of acidification and organic acid metabolites.

Electro fermentation conditions were mimicked using a modest oxidative potential (+0.4 V versus Ag/AgCl) and 20 μ M 2-hydroxy-1,4-naphthoquinone (HNQ), a redox mediator. Although HNQ increased current output and electrochemical responsiveness, it had little effect on bacterial growth. The inhibitory impact of *L. plantarum* on *S. aureus* was enhanced by electrochemical stimulation, particularly in co-culture biofilms grown on conductive screen-printed electrodes. This was demonstrated by fluorescence microscopy and verified by image analysis, which revealed a 70% decrease in biofilm coverage.

These results highlight the possibility of combining nanoparticles and electrochemical stimulations to enhance the production of natural antibiotics and show that *L. plantarum* is a strong natural antimicrobial, particularly in acidic and anaerobic environments. This integrative strategy shows promise for developing advanced probiotic-nanomaterial hybrid therapies to combat biofilm-forming, drug-resistant pathogens on biomedical surfaces.

Keywords: *Lactobacillus plantarum*, *Staphylococcus aureus*, antimicrobial resistance, co-culture, compound medium, electro fermentation, biofilm inhibition, cell-free supernatant

O-05 Application of coarse-grained DNA mathematical model for studying the genesis of additional open state zones in the extended polyQ tract of the ATXN2 gene

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Abstract: The ATXN2 gene is located on chromosome 12q24.1 and encodes the ataxin-2 protein, which is involved in the regulation of RNA metabolism, protein synthesis, and intracellular signaling. The polyQ tract encoding glutamine can expand, leading to various neurodegenerative diseases. CAA interrupts play an important role in the stabilization of the polyQ tract in the ATXN2 gene. However, CAA interruptions may be associated with other neurodegenerative conditions such as Parkinsonism. It is believed that the mechanisms of occurrence of these diseases are associated with the possible formation of non-canonical configurations (hairpins, etc.) in the extended polyQ tract. At the same time, hairpins can occur only in areas of open states.

Modeling of open states of DNA under the influence of the torsion moment is a key aspect of studying supercoiling, topoisomerase activity, and replication/transcription mechanisms. The process of formation and dynamics of open state zones in a double-stranded DNA molecule is largely determined by its mechanical properties.

Coarse-grained models allow efficient investigation of these processes without the lengthy large-scale calculations required for atomic detail. The angular model of the DNA molecule is based on the analogy between a double-stranded DNA molecule and a mechanical system consisting of two chains of interconnected pendulums.

In this paper, mathematical modeling methods have been used to study the stability (the probability of additional zones of open states in the polyQ tract, prone to hairpin formation) of the polyQ tract in the presence of CAA interruptions, depending on their localization. It has been found that interruptions located near the center of the polyQ tract significantly reduce their stability, and those located near its boundaries can both reduce and increase the stability of the polyQ tract. At the same time, there is a certain asymmetry: CAA interrupts located near the left border of the polyQ tract have a more stabilizing effect than CAA interruptions located near the right border. In addition, the angular model makes it possible to calculate the localization of mechanical energy in a DNA molecule under external influence. This makes it possible to predict the places of origin of open states.

One of the possible further applications of the model may be to calculate the effect of deuterium (D/H substitution in hydrogen bonds between nitrogenous bases) on the occurrence of additional OS zones in the region of CAG repeats. In addition, a promising area is the study of other genetically determined diseases using the developed approaches.

Funding: The research is carried out with the financial support of the Russian Science Foundation and the Kuban Science Foundation in the framework of the scientific project Num. 24-14-20014, <https://rscf.ru/en/project/24-14-20014/> (accessed on 11 November 2024).

Keywords: *Coarse-grained DNA mathematical model, ATXN2, open states of DNA, trinucleotide repeat diseases, CAA interrupts*

O-06 Biosynthesis and characterisation of silver nanoparticles using *Bacillus subtilis* and their commercial formulation

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Abstract: Silver nanoparticles (AgNPs) are widely recognized for their antimicrobial, antioxidant, and catalytic properties. However, traditional synthesis methods often involve toxic chemicals and high energy consumption, making them less suitable for sustainable applications. In this study, we employed *Bacillus subtilis*, a GRAS-status bacterium, for the biosynthesis of AgNPs through a green, cost-effective method. The process involved incubating the cell-free supernatant of *B. subtilis* with silver nitrate (AgNO_3), which led to a visible color change indicating nanoparticle formation. Characterization techniques including UV-Vis, FTIR, SEM, TEM, and XRD confirmed the formation, morphology, size, and crystalline nature of the synthesized AgNPs.

LC-MS profiling of the bacterial extract identified key metabolites such as surfactin, fengycin, subtilin, and bacilysin, which are likely involved in the reduction and stabilization of silver ions. The AgNPs were then formulated into antimicrobial gels and coatings, which exhibited strong inhibitory activity against selected pathogens. Cytotoxicity and stability assessments supported their potential for safe biomedical applications. This study highlights *Bacillus subtilis* as a reliable biological platform for sustainable nanoparticle synthesis and introduces a scalable pathway for commercial product development in the field of green nanotechnology.

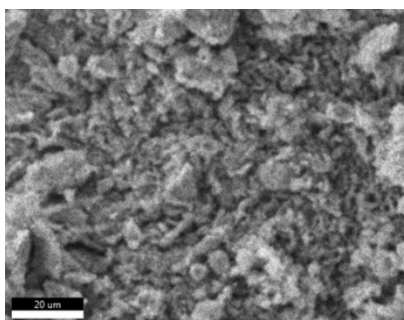


Fig: FE-SEM Analysis of *bacillus subtilis* nanoparticle

Keywords: Silver nanoparticles, *Bacillus subtilis*, biosynthesis, antimicrobial gel, green nanotechnology

O-07 Engineering small modular recombinant antibodies for chromatin studies

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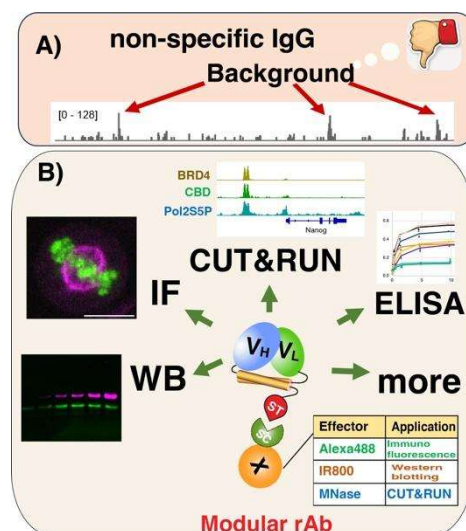
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Abstract: Antibodies are indispensable tools in our investigations of transcriptional regulation and cell fate decisions. However, conventional IgG antibodies (~150 kDa) pose several limitations, including non-specific background, batch-to-batch variability, and limited molecular customization. For instance, negative control IgGs often produce artificial “peaky” signals in the profiling CUT&RUN assays due to cross-linking via Fc domains or secondary antibodies, which can mislead interpretation of chromatin-binding profiles (Fig. A).

To overcome these limitations, we developed small, modular recombinant antibodies (rAbs) in either Fv-clasp (~40 kDa) or nanobody (~15 kDa) formats. These rAbs are structurally stable, reproducibly expressed in *E. coli*, and are easy to protein engineer. We further enhanced their versatility by incorporating the SpyTag-SpyCatcher system, allowing rapid labeling of rAbs with functional molecules (e.g., enzymes, fluorophores). Specifically, SpyTag (~1.3 kDa) is fused to rAbs, enabling modular decoration with SpyCatcher-conjugated effectors for different applications (Fig. B).

Our modular rAbs demonstrated excellent performance across various applications, including Western blotting and immunofluorescence, offering high signal-to-noise ratios and eliminating the need for secondary antibodies. In CUT&RUN, rAbs consistently outperformed conventional IgGs in resolution, specificity, reproducibility, and target accessibility. Given their scalable production and reliable performance, our modular rAbs hold strong potential for preparative-scale applications such as chromatin immunoprecipitation for proteomics and multiplex high-resolution applications.

Keywords: modular recombinant antibody, SpyTag-SpyCatcher conjugation system, antibody's reproducibility, enhanced resolution for chromatin profiling, animal-free production



O-08 Enhanced Superconductivity in Pb₂Au Alloy on Pb(111)

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Abstract: Superconducting materials are fundamental to the development of nano-device technology, as illustrated by their applications in magnetic resonance imaging (MRI) and nuclear magnetic resonance (NMR) systems. In this work, we deposited Au on Pb(111) substrate and studied its superconducting properties below the critical temperature T_c . Lead is well known as a superconducting element, with a transition temperature T_c of about 7.2°K, whereas gold (Au) is not superconducting. Interestingly, Pb₂Au alloy exhibits superconducting properties with a larger superconducting gap compared to the Pb(111) substrate, indicating an enhancement in superconductivity. The electronic structure of the surface was characterized by using low energy electron diffraction (LEED), scanning tunneling microscope (STM) and angle-resolved photoemission spectroscopy (ARPES). Furthermore, the superconducting gap is examined by scanning tunneling spectroscopy (STS) at low temperature.

Keywords: Superconducting materials, nano-device, alloy, superconducting gap, enhanced superconductivity

O-09 From UV Activation to Surface Binding: Charge Transfer Strategies in SERS

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Abstract: Surface-enhanced Raman scattering (SERS) enables ultrasensitive, label-free molecular detection, with performance largely dictated by the substrate's ability to amplify Raman signals. While noble metals provide strong electromagnetic enhancement via localized surface plasmon resonance, coupling them with semiconductors introduces additional chemical enhancement through efficient charge transfer. Our recent work examines TiO₂/Ag, MnO₂/Ag, and ZnO/Ag nanocomposites, each following distinct pathways. TiO₂/Ag employs a semiconductor–metal–substrate route via the photoinduced enhanced Raman spectroscopy (PIERS) effect, where UV-induced oxygen vacancies in TiO₂ facilitate hot-electron transfer from Ag to the analyte. Conversely, MnO₂/Ag and ZnO/Ag follow a metal– semiconductor–substrate route, with analyte chemisorption on the semiconductor promoting charge transfer from Ag through the semiconductor. These mechanisms yield sub-nanomolar detection limits and high enhancement factors. This presentation reviews mechanistic insights and performance benchmarks from these systems, offering design principles for ultra-sensitive semiconductor–metal SERS platforms in environmental, biomedical, and agricultural sensing.

Keywords: *Surface-enhanced Raman scattering (SERS), semiconductor–metal nanocomposites, charge transfer mechanism, PIERS effect, TiO₂/Ag, MnO₂/Ag, ZnO/Ag.*

O-11 Influence of Surface Chemistry on the Toxicity of Thiolated and PEGylated Organosilica Nanoparticles

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Abstract: Silica nanoparticles are among the promising materials for biomedical applications, particularly in drug delivery and diagnostics. However, pure silica nanoparticles may exhibit intrinsic toxicity, and PEGylation is therefore considered a viable strategy to reduce their toxicological impact and improve bioavailability.

In this work, we examined the toxicological characteristics of thiolated and PEGylated organosilica nanoparticles that were synthesised by self-condensation from (3-mercaptopropyl)trimethoxysilane (MPTS). One significant benefit of these nanoparticles is their surface thiol groups, which are easily exploited for further functionalization or for drug transport to mucosal tissues. Given the well-established mucoadhesive properties of thiol groups, thiolated organosilica nanoparticles offer a promising platform for mucosal drug delivery. However, mucoadhesion alone does not ensure the suitability of a material for biomedical applications. Therefore, in order to determine if surface modifications have a substantial impact on the characteristics of thiolated organosilica nanoparticles, we evaluated their physicochemical characteristics and toxicological profile.

We investigated the toxicological effects of PEGylated (SiNP-PEG5000) and thiolated (SiNP-SH) nanoparticles using low- and high-molecular-weight polyethylene glycol in a variety of cell cultures, human blood, and animal models. Prior to and during the nanoparticles treatment, we also examined the permeability and biophysical-biomechanical properties of the cells.

Collectively, our findings demonstrate that surface modifications of organosilica nanoparticles significantly influence their physicochemical properties and modulate cellular responses. This work provides a comprehensive toxicological assessment of thiolated and PEGylated organosilica nanoparticles, uncovering how surface modifications can influence their behaviour and advancing knowledge of their potential uses in biomedicine.

Keywords: *organosilica, PEGylation, thiolated nanoparticles, surface modification, cytotoxicity*

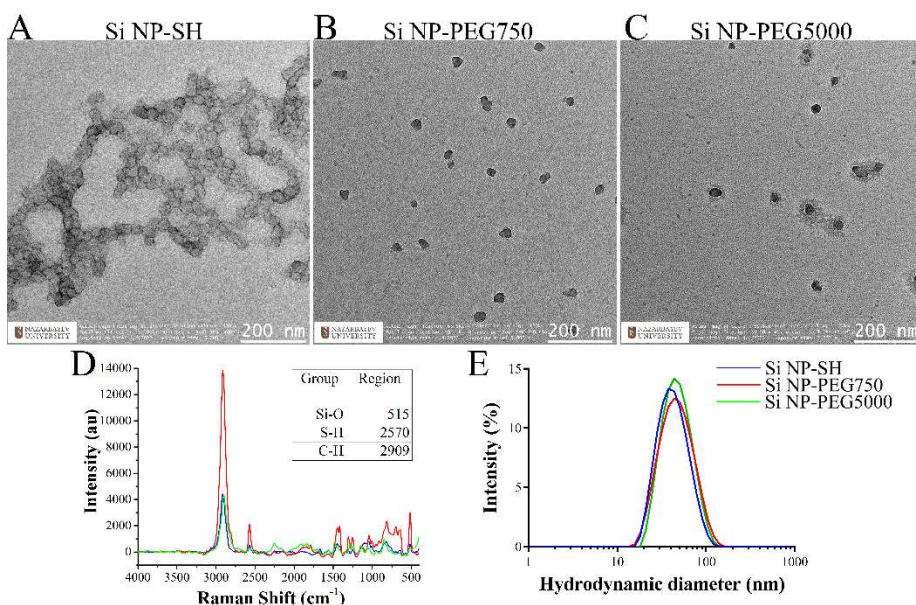


Figure: Physicochemical characterisation of thiolated and PEGylated organosilica nanoparticles: (A–C) TEM images of SiNP-SH, SiNP-PEG750, and SiNP-PEG5000; (D) Raman spectra; (E) hydrodynamic size distribution in water.

O-12 Myco-engineered silver nanoparticles from *Penicillium oxalicum* exhibits *in vitro* anti-proliferative activity and potentially mediates *in vivo* breast tumor regression

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Abstract: Fungal endophytes being rich producers of pharmaceutically important bioactive compounds have been emerged as a potential candidate in the field of nanobiotechnology extending their applications in the biomedical field. The present study focuses on fabrication of green silver nanoparticles using aqueous extract of *Penicillium oxalicum* (POAgNPs), a fungal endophyte associated with a medicinal plant *Amoora rohituka*, and evaluation of their *in vitro* and *in vivo* anti-breast cancer activity. The synthesis of POAgNPs was validated by different characterization techniques where sharp UV–visible spectra was observed at 420 nm, crystalline nature was revealed by XRD analysis, FTIR analysis showed possible functional groups of fungal biomolecules involved in the reduction and stabilization of POAgNPs and, average size of NPs as 17 nm were revealed by AFM, TEM, and FESEM. The drug release study of POAgNPs showed higher release kinetics at low pH that corresponds to tumor microenvironment. The potential anti-proliferative activity of POAgNPs was revealed against human breast cancer cells, MDA-MB-231 and MCF-7 in a dose-dependent manner and intracellular ROS generation has also been reported in POAgNPs treated breast cancer cells (BCs). The real-time cytotoxic activity of POAgNPs was studied through cell impedance measurement and quantitative multivariate analysis for POAgNPs induced cytotoxic effects in BCs was studied through high content imaging platform that showed internalization of POAgNPs inside BCs and alteration in morphological parameters in a dose-dependent manner. The molecular study showed the differential expression of apoptosis-related genes in BCs after treatment with POAgNPs. The genotoxicity profiles of POAgNPs were demonstrated against *in vivo* animal models and no signs of toxicity were observed. Further, *in vivo* tumor regression potential of POAgNPs was performed using animal models and photoacoustic imaging showed regression of breast tumor in animals after POAgNPs administration. The histopathological and biochemical examination revealed the tumor regression following treatment with POAgNPs. Moreover, alteration in metabolic parameters were studied using plasma and breast tumor tissue homogenate that showed decreased glucose uptake and lactate dehydrogenase release in POAgNPs treated groups. The homeostatic control over the redox

status was reported in treated animals as reported through decreased level of lipid peroxidation and nitric oxide production and increase in reduced glutathione level. The alteration in expression of genes was reported in POAgNPs treated animals revealing upregulation of apoptosis-related genes including *P53* and *CASPASE-8* and downregulation of anti-apoptotic gene *BCL-XL* and glucose transporter gene *SLC2A1*. The fold-change in Caspase-3 activity was found in treated animals that shows the alteration in protein expression. The green synthesized POAgNPs thus showed significant potential against regression of breast tumor and therefore, the study necessitates further exploration to dissect molecular pathways and subsequent clinical trials.

Keywords: *Fungal endophytes, POAgNPs, Breast cancer, cytotoxic activity, apoptosis, tumor regression*

POSTER PRESENTATION

PP-01 Fabrication of TiO₂ Nanorods on different substrates for sensor application

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Abstract: In this study, rutile-phase TiO₂ nanorods were synthesized via a hydrothermal method on diverse substrates and utilized for heavy metal sensing based on fluorescence. Specifically, the nanorods were grown on two distinct types of substrates: anatase-phase TiO₂ thin films deposited via pulsed electron deposition (PED) and fluorine-doped tin oxide (FTO) conductive glass substrates. A notable variation in the morphology and nanostructure of the TiO₂ nanorods was observed depending on the underlying substrate. Nanorods on FTO substrates exhibited vertically aligned growth with uniform distribution, while those on PED-derived anatase-phase TiO₂ thin films tended to aggregate into flower-like clusters. Furthermore, the impact of H⁺ ion concentration in the precursor solution on the growth mechanism was systematically investigated. Modulating H⁺ ion concentration significantly influenced both nanorod thickness and surface coverage density on the anatase TiO₂ substrate, indicating a strong correlation between solution acidity and growth behavior. Fluorescence-based sensing experiments employing rutile nanorods grown on PED-deposited anatase TiO₂ films demonstrated outstanding performance in heavy metal ion detection, achieving limits of detection of 0.12 μM for Fe³⁺ and 0.32 μM for Pb²⁺, with corresponding linear response ranges of 0.05–1 μM and 0.005–1 μM , respectively [1]. These findings imply the high sensitivity and reliability of the developed sensor platform, highlighting the promising potential of nanostructured TiO₂ materials for heavy metal ion sensing applications.

Keywords: TiO₂ anatase/rutile heterojunction, Pulsed electron deposition, Hydrothermal synthesis, Fluorescence sensing, Heavy metal ion detection, Dopamine sensor.

References:

[1] Q.-D. Dao, *et al.*, submitted to *Applied Surface Science*.

PP-02 Identification of Novel KRAS G12C Inhibitors for Lung Cancer Via High-Performance Computing-Guided Virtual Screening

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Abstract: Lung cancer is one of the deadliest cancers, with millions of people diagnosed worldwide each year. Despite significant advances in diagnostic and treatment technologies, it remains a major challenge in modern medicine. Lung cancer is characterized by the abnormal and uncontrolled growth of cells in the lungs, particularly within the bronchial tubes. Non-small cell lung cancer (NSCLC) accounts for approximately 85% of all lung cancer cases, and among these, the KRAS G12C mutation is one of the most frequent. This mutation keeps the KRAS protein permanently active, driving uncontrolled cell growth and tumor formation. Sotorasib and adagrasib are small-molecule inhibitors that specifically target KRAS G12C and are approved by the United States Food and Drug Administration (FDA) for cancer therapy. However, most patients with KRAS G12C-mutant NSCLC develop resistance, and the effectiveness of these drugs typically diminishes within a year. Moreover, traditional small-molecule screening methods are often laborious, costly, and limited by the number of compounds that can be tested. Therefore, there is an urgent need for new strategies to identify KRAS G12C inhibitors. In this study, we leverage high-performance computing to virtually screen millions of compound structures, aiming to identify small molecules that bind to KRAS G12C with affinity equal to or greater than that of sotorasib or adagrasib. To this end, we first extracted the KRAS G12C protein structure from the Protein Data Bank (PDB code: 5YXZ). To prepare the receptor for ligand screening, we removed the original ligand (quinazoline) as well as all water molecules. Hydrogens were subsequently added, and Kollman charges were assigned. The ligand docking area, encompassing the G12C mutation site, was defined as the grid box for molecular docking using the AutoDock Vina algorithm. To compare binding affinities, we assessed the binding of sotorasib and adagrasib to KRAS G12C using AutoDock Vina, with these compounds serving as reference ligands for evaluating binding efficiency. We then performed virtual screening of KRAS G12C using

AutoDock Vina within our established pipeline on high-performance computing clusters, utilizing approximately four million compound structures from the ZINC database. Through this process, we identified a repertoire of compounds with higher predicted binding affinity than both sotorasib and adagrasib. We are currently expanding our screening pipeline to identify the most promising compounds with the highest binding affinities, and we plan to test the anticancer activity of these candidates on NSCLC cell lines harboring KRAS G12C mutations, as well as on primary cancer cells derived from NSCLC patients with KRAS G12C. Our overarching goal is to establish additional KRAS G12C inhibitors, paving the way for further pharmacological optimization and eventual clinical trials. Ultimately, this research holds the promise of significantly improving survival rates and quality of life for NSCLC patients, who currently face limited treatment options and poor prognoses.

Keywords: *Non-small cell lung cancer, KRAS G12C, High-Performance Computing, Molecular docking, small molecule inhibitors*

PP-03 Fabrication of vertically aligned TiO₂ nanorod for simultaneous detection and remediation of environmental pollutants

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Abstract: This study presents fabrication of vertically aligned TiO₂ nanorods through simple hydrothermal techniques, aimed at developing an integrated system for the detection and treatment of environmental pollutants. Through precise control of proton (H⁺) concentration in the precursor solution, we have successfully eliminated undesirable TiO₂ nanostructures, such as flower-like structure, thereby producing rutile-phase TiO₂ nanorods with perfect vertical alignment and an average diameter of 70 nm on fluorine-doped tin oxide substrates. The fluorescence sensors utilizing these synthesized TiO₂ nanorods exhibit a low limit of detection of 0.16 μM for Fe³⁺ ions and 0.09 μM for Pb²⁺ ions, with corresponding linear detection ranges of 0.03 μM - 1 μM and 0.002 μM - 0.05 μM, respectively [1]. Notably, the integration of TiO₂ nanorods with Au nanoparticles creates highly efficient surface-enhanced Raman scattering (SERS) substrates. Characteristic Raman peaks at 1623.3 cm⁻¹ appear distinctly in the presence of 10⁻¹¹ M methylene blue and disappear completely after 50 minutes of UV irradiation, demonstrating the superior potential of Au/TiO₂ SERS substrates for detecting and degrading organic pollutants. Furthermore, our research focuses on the morphology and crystal structure of TiO₂ nanorods to elucidate the influence of proton (H⁺) concentration on the growth mechanism.

Keywords: *TiO₂ nanorod; Hydrothermal method; sensor; fluorescence; SERS.*

References:

[1] Q.-D. Dao, *et al.*, submitting to *Journal of Physics D: Applied Physics*.

PP-04 Evaluating the Effect of Proteins on Enhancing Preservation and Oral Administration Efficiency in Phage Therapy via Extrusion Encapsulation

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Abstract: Bacteriophage therapy offers a promising solution for combating multidrug-resistant pathogens in aquaculture. However, phage effectiveness is often limited by rapid inactivation under harsh conditions, particularly the low pH of gastric fluids during oral administration. To overcome this, encapsulation strategies are essential to protect phages and maintain their activity. Encapsulated by extruding methods using pure alginate and animal-derived proteins like whey protein isolate (WPI) are effective but face limitations due to cost. This study proposes a novel approach using soy protein isolate (SPI), a plant-based, cost-effective alternative—combined with food-grade alginate to develop a protective delivery system. In simulated gastric fluid (SGF), SPI-alginate beads preserved phage titers at 10^7 PFU/mL for 120 minutes. In contrast, alginate-only beads showed a 2-log reduction (10^7 to 10^5 PFU/mL), and free phages dropped to 10^2 PFU/mL within 200 seconds. These results demonstrate that SPI-alginate encapsulation effectively protects bacteriophage stability. Moreover, this plant-based system is both efficient and affordable, highlighting SPI's potential for sustainable phage delivery in aquaculture.

Keywords: Bacteriophage, encapsulation, soy protein isolate, oral administration, aquaculture.

PP-05 **Studies on the impact of the core-shell structures on the optical characteristics of Au@Cu₂O nanoparticles**

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Abstract: Nanoparticles (NPs) with metal@dielectric core@shell, nano-sized dimensions, and local surface plasmon resonance peaks (LSPR) must play a vital role owing to their optical interaction and comprehensive array of applications in several fields, including information transmission, biomedicine, and other advanced technologies. This work examines the optical characteristics of core/shell nanoparticle structures that can be regulated via aggregation. These structures have Au nanoparticles (NP) measuring 16.6 nm in diameter, while the shell thickness ranges from 24.6 ± 3.6 to 9.0 ± 1.7 nm. The absorption and scattering spectra of the gold core-Cu₂O shell were analysed using the boundary element method (BEM). The absorption of cross-sections over various wavelengths of light was determined by solving the Maxwell equations. Both Ox- and Oz-axis polarizations of an incident plane wave are used to determine the core-shell Au@Cu₂O nanoparticles' field enhancement. Factors such as the core-shell ratio, the particle's morphologies, and the spacing between the particles are taken into consideration to evaluate how particle structures influence their optical properties. The particle system's distribution and organization were also considered, along with an analysis of the impact of the particle arrangement and distribution within the particle system. The similarity between the calculation and experimental results underscores the accuracy of our simulation model.

Keywords: *Au@Cu₂O nanoparticles, core-shell metal nanoparticles, boundary element method (BEM), surface plasmon resonance peaks (LSPR)*

PP-06 Enhanced non-enzymatic optical glucose sensing using ZnO/CuO nanocomposites and FOX assay

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Abstract: The development of reliable and efficient glucose sensors is essential for managing diabetes and preventing its complications. In this study, we report a novel optical glucose sensor combining ZnO/CuO nanocomposites and the ferrous oxidation-xylenol orange (FOX) assay. ZnO/CuO nanocomposites were synthesized using a two-step hydrothermal method. The synthesized nanocomposites were characterized using scanning electron microscopy (SEM), X-ray diffraction (XRD), and Raman scattering to determine their morphological and structural properties. The sensor exhibits remarkable sensitivity (20.2%/mM) in the glucose concentration range of 0-4 mM, a low detection limit of 0.08 mM, and excellent selectivity against common interfering substances in other sugars. Our results underscore the ability of ZnO/CuO nanocomposites for life science applications.

Keywords: ZnO/CuO, nanocomposites, hydrothermal, glucose sensor, FOX assay.

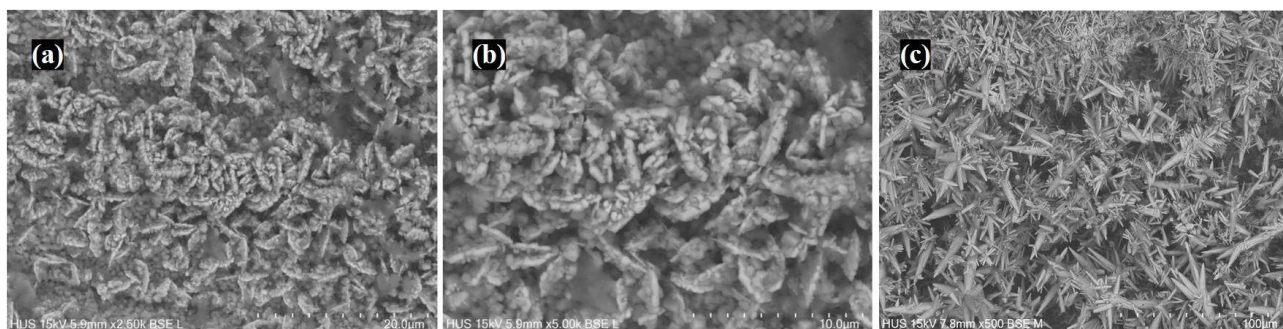


Figure 1: SEM images of (a, b) CuO nanoparticles and (c) ZnO/CuO nanocomposites.

PP-07 Atomistic Insights into Charge Transfer Mechanisms in DNA Biosensor on CeO₂ (111)

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Abstract: Understanding the charge transfer (CT) mechanism at bio-inorganic interfaces is essential for advancing the design of DNA – based electrochemical biosensors. In this work, we employ density functional theory (DFT) with Hubbard U corrections to investigate the redox behavior of ferrocyanide, Fe(CN)₆, at the ceria surface, CeO₂ (111), both in the absence and presence of DNA nucleobases. We develop a quantitative framework to evaluate the CT energy and CT transition rate based on the alignment of Fe(5d) and Ce(7f) orbital energies. Our simulations reveal that the presence of a single cytosine, guanine, or their pair significantly alters the CT mechanism by preventing direct Fe(CN)₆ – CeO₂ (111) binding, modifying orbital energies, and increasing the CT energy. The differences in CT energy between single – nucleobase and base – pair configurations support experimentally observed redox potential shifts during the DNA hybridization. Notably, the Fe(CN)₆@C@CeO₂(111) configuration exhibits an enhanced CT transition rate due to proton transfer from cytosine, identifying cytosine – rich single – stranded DNA as an optimal probe for biosensing applications. These insights provide an atomistic foundation for the rational design of sensitive and selective DNA biosensors.

Keywords: Charge transfer mechanism, DNA-based electrochemical biosensor, Density functional theory (DFT), CT energy, DNA hybridization.

PP-08 Biopolymer Film Embedded Nanoparticles for Antimicrobial Application and Fresh Fruit Preservation

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Abstract: In this study, an intelligent carboxymethyl cellulose (CMC)-based biopolymer film incorporating silver (Ag) and zinc oxide (ZnO) nanoparticles was fabricated for the preservation of fresh avocados. Scanning electron microscopy (SEM) and optical microscopy analyses revealed that the CMC–ZnO–Ag film possessed a thickness of less than 20 μm , with nanoparticles uniformly distributed within the CMC matrix. CMC–ZnO–Ag demonstrated over 95% inhibition against harmful microorganisms, including *Escherichia coli* (*E. coli*), *Staphylococcus aureus* (*S.aureus*), and a range of yeasts and molds. As a proof of concept, CMC–ZnO–Ag was applied to avocado preservation, effectively maintaining fruit freshness for up to 35 days. These findings highlight the film’s potential as an active packaging material for protecting fruits and other perishable foods from harmful microbial contamination.

Keywords: Carboxymethyl cellulose CMC, ZnO nanoparticles, Ag nanoparticles, antimicrobial, fruit preservation

PP-09 Research and fabrication of nanoparticle-incorporated coating films for preserving Dak Lak traditional durian

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Abstract: In recent years, Vietnamese fruits have experienced significant growth in both production and variety, particularly durian – one of the most economically valuable fruits. However, due to its perishable nature and a ripening period of only 2 – 4 days, durian faces numerous challenges in storage and long-distance transportation, especially when exported to distant markets. In this study, we focused on developing and optimizing a film-forming gel solution containing nanomaterials and biopolymers to extend the shelf life of Dak Lak traditional durian. This solution is based on the combination of the biopolymer Carboxymethyl Cellulose (CMC) with advanced nanomaterials such as nano ZnO and nano Ag. The CMC–ZnO–Ag coating demonstrated an inhibitory effect of over 95% against several harmful microorganisms, such as *Escherichia coli* (E. coli), *Staphylococcus aureus* (S. aureus), and certain yeasts and molds. The research results indicate that this coating can extend the shelf life of durians up to 15 days under controlled conditions, reduce spoilage rate, minimize weight loss, slow down the ripening process, and maintain nutritional quality. The application of nanopolymer technology not only enhances the export potential of Đắk Lắk durians but also contributes to the sustainable development of Vietnam's agricultural sector.

Keywords: CMC, nano ZnO, nano Ag, coating films, preservation

PP-10 Development of a fluorescent sensor for dopamine sensing

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Abstract: As of 2025, measuring dopamine levels in the body has become a significant area of research in medical and pharmaceutical sciences due to the important role of dopamine in the nervous system signaling processes. Therefore, precise monitoring of the concentration of dopamine is always of high interest for future medical applications. In this work, we succeeded in synthesizing the nanocomposite of g-C₃N₄/ZnO NRs by a simple, low-cost method. The surface morphology and the optical properties of the nanocomposite material were considered. The nanocomposite was then used for the development of a dopamine fluorescent sensor. The working principle of the sensor is based on the fluorescent quenching of the sensor concerning the increase of dopamine concentrations. Other characteristics of the sensor such as limit of detection and working range were also investigated in detail.

Keywords: Dopamine, g-C₃N₄/ZnO, fluorescent quenching, nanocomposite.

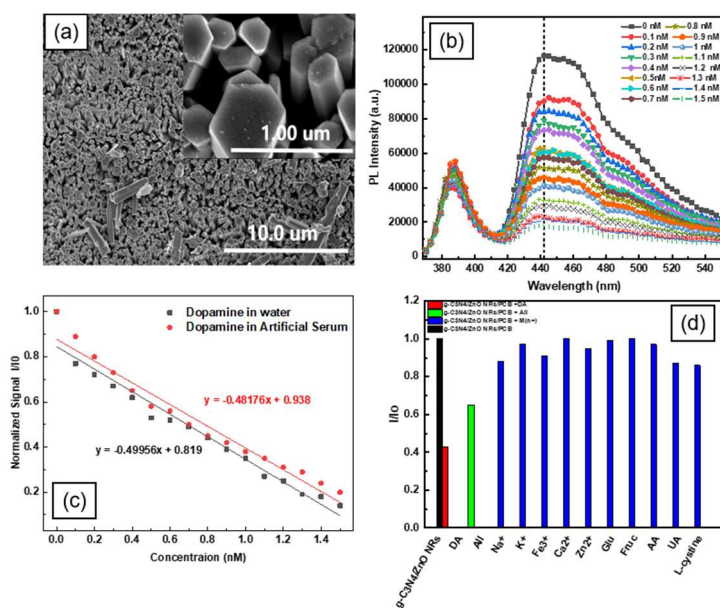


Figure: a) surface of g-C₃N₄/ZnO/PCB, b) Fluorescence quenching spectrum of g-C₃N₄/ZnO increasing dopamine concentration, c) Calibration curve and sensitivity of fluorescence sensor, d) sensor selectivity

PP-11 **Fabrication of Whispering Gallery Mode Microlasers Based on Biocompatible Materials and Silica Nanoparticles**

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Abstract: This study focuses on the fabrication and investigation of the optical properties of Whispering Gallery Mode (WGM) microlasers based on the biocompatible BSA–RhB material integrated with silica nanoparticles. The microspheres incorporating silica nanoparticles, with diameters ranging from 25–35 μm , exhibit high lasing efficiency and strong resistance to degradation in common environments. The results show that pure BSA–RhB microspheres tend to emit WGM lasing with a narrow spectrum, low threshold, and visible-range emission. Upon the incorporation of silica nanoparticles, the emission mechanism shifts toward random lasing, with enhanced emission intensity and reduced threshold due to increased scattering and mode coupling. Varying the silica nanoparticle content and the microsphere size leads to wavelength shifts, changes in spectral characteristics, and influences optical stability. Lasing signals are also observed when the microspheres are placed in biological environments. These findings demonstrate that the hybrid BSA–RhB–Silica material holds great potential for applications in biosensing, environmental monitoring, and tunable photonic devices.

Keywords: *Whispering Gallery Mode, BSA–RhB microspheres, silica nanoparticles, random laser, biosensing*

PP-12 **UV photo-conductive glucose**

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Abstract: In this study, glucose concentration is determined using an electrical method based on ZnO nanorods (ZnO NRs) through resistance changes. Using a one-step hydrothermal method, ZnO nanorods are successfully synthesized on gold electrodes. The morphological surface of ZnO NRs is investigated using SEM measurement, with an average diameter of the ZnO nanorods is 0.888 ± 0.05 μm that are demonstrated from the SEM image. The minimal detection of the method is 0.01 mM, and the measurement range is 0.1-10 mM. To highlight the specificity, we tested various sugars, and the results showed that our method has high specificity for glucose. This demonstrates that the electrical glucose sensor using ZnO material has great potential for practical applications.

Keywords: *Electrical glucose sensing based on ZnO nanorods*

PP-13 Investigating the binding of agonists to the stability of μ -opioid receptor

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Abstract: Opioid agonists expressing analgesia are usually followed by adverse reactions such as heart failure, respiratory depression, constipation, etc. Agonist binding to μ -opioid receptors (μ OR) can activate two intracellular signaling pathways: (i) the G protein signal is responsible for alleviating pain; (ii) β -arrestin results in unwanted side effects. Here, we utilize recent advances in computational power and molecular dynamics (MD) simulations to analyze and evaluate the influences of unbiased (Morphine – M6G) and biased (TRV130) compounds of the G protein signal, on the structural stability and functions of the μ OR receptor. We have identified that M6G with hydroxyl groups, forms Hydrogen bond and electrostatic interactions with key residues in the catalytic site of the μ OR receptor, whereas TRV130 prefers binding by hydrophobic and van der Waals interaction types. The binding to M6G leads to the higher flexibility of the μ OR's TM VII which is known to activate the β -arrestin signal, while this TM VII is more stable in the TRV130- μ OR complex. Additionally, the allosteric pockets of the Sodium (Na^+) ion are different in these μ OR complexes. Taken together, these studies may provide new avenues for the design of biased opioids with appropriate efficacy.

Keywords: μ -opioid receptors, molecular dynamics (MD) simulations, Morphine – M6G, TRV130, Sodium (Na^+) ion

PP-14 Antimicrobial activity of PLA/PEG@Ag nanofiber membranes prepared via electrospinning

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Abstract: Electrospun nanofiber membranes composed of polylactic acid (PLA), polyethylene glycol (PEG), and silver nanoparticles (AgNPs) were successfully fabricated and systematically investigated for their antimicrobial activity. The influence of electrospinning parameters, including polymer solution concentrations (8-10 wt%), solvent mixture ratios N, N-dimethylformamide/ chloroform (80/20-70/30), and PLA to PEG@Ag weight ratios (95/5-80/20) on fiber morphology and average diameter was characterized using scanning electron microscopy (SEM). Optimal conditions were identified with a 9 wt% PLA/PEG@Ag solution (PLA/PEG@Ag = 95/5) in a DMF/chloroform system (75/25), yielding uniform, bead-free nanofibers with an average diameter of approximately 400 nm. The antibacterial test demonstrated that incorporating AgNPs into the PLA/PEG@Ag nanofibrous membrane endowed it with pronounced antimicrobial activity against *E. coli* and *MRSA*. Furthermore, shelf-life studies on strawberries showed that PLA membrane modified with PEG@Ag effectively inhibited microbial growth and delayed spoilage. These findings highlight the dual potential of PLA/PEG@Ag nanofiber membranes, not only as sustainable active food packaging materials but also as promising candidates for biomedical applications, such as antimicrobial wound dressings and infection-preventive coatings.

Keywords: Electrospinning, packaging materials, silver nanoparticles, polyethylene glycol, polylactic acid.

PP-15 Shape memory performance and antibacterial properties of electrospun PCL/PEG/BP nanofiber membranes

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Abstract: In this study, poly(ϵ -caprolactone) (PCL)/polyethylene glycol (PEG) nanofiber membranes incorporating different amounts of benzophenone (BP) were fabricated via electrospinning and subsequently crosslinked under ultraviolet irradiation ($\lambda \approx 365$ nm) to introduce shape memory functionality. The shape memory network was formed through physical net points provided by PEG and chemical crosslinks induced by BP, which contributes to enhancing both the shape memory performance and the antibacterial activity of the PCL/PEG/BP fibrous membranes. Shape memory behavior varies with BP content under thermal activation, with membranes containing 5 wt% BP exhibiting optimal performance. These membranes achieved fixation and recovery ratios exceeding 98% and 90%, respectively, after 15 minutes at 56 °C. The temperature-dependent recovery behavior suggests potential applications as passive indicators in smart monitoring systems. The membranes were characterized by Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), and differential scanning calorimetry (DSC) to evaluate their chemical structure, morphology, and thermal stability. Additionally, the PCL/PEG/BP membranes exhibited strong antibacterial activity, effectively inhibiting *MRSA* and eliminating *E.coli*. These findings suggest that the developed PCL/PEG/BP membranes provide a new class of shape-memory materials with great potential for food packaging applications, paving the way for their integration into smart monitoring systems.

Keywords: Shape memory materials, electrospinning, benzophenone, chemical crosslinks, poly(ϵ -caprolactone).

PP-16 Sensitive Detection of Trace Antibiotics Using Surface-Enhanced Raman Scattering (SERS) Based on Al-doped ZnO Nanorods Decorated with Noble Metal Nanoparticles

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Abstract: Surface-enhanced Raman scattering (SERS) is a powerful analytical technique that offers multiple advantages, including the ability to detect trace amounts of organic compounds at extremely low concentrations and relatively easy measurement procedure. The two basic mechanisms of SERS are electromagnetic enhancement (EM) and chemical enhancement (CM) which coexist in most SERS systems. In this research, Al-doped ZnO nanorods with various Al-doping concentrations were grown on glass substrates using the chemical bath deposition method. The incorporation of Al³⁺ into the ZnO structure increases the carrier concentration and introduces more defects, which in turn enhances the performance of CM in SERS. The Noble metal nanoparticles with an average diameter of 20 nm, decorated on Al-doped ZnO nanorods, combined with the numerous “hot spots” and large effective surface area of the nanorods, produce highly sensitive SERS substrates through the EM. The SERS substrate with the optimal Al-doping concentration, consisting of Al-doped ZnO nanorods approximately 3 μ m in length and 500 nm in diameter, was used to detect antibiotics in seafood. Raman measurements demonstrated that this SERS method can detect antibiotics at concentrations as low as 0.005 ppm.

Keywords: *SERS, Al-doped zinc oxide nanorods, noble metal nanoparticles, antibiotic detection.*

PP-17 Signal enhancement of polymerase chain reaction (PCR) reaction using low-dimensional structured gold nanomaterials for the detection of tobacco mosaic virus

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Abstract: Tobacco mosaic virus (TMV) is one of the most economically important plant viruses in Việt Nam, causing severe losses in tobacco, tomato, pepper, and other solanaceous crops. Early and accurate detection is essential for disease management, yet conventional PCR methods are often constrained by sensitivity, specificity, and the need for laboratory infrastructure. Nanoparticle-assisted PCR (nanoPCR) represents an emerging approach that exploits the unique thermal and surface properties of nanoparticles to enhance amplification. In this study, we developed a nanoPCR assay using gold nanoparticles (AuNPs) to improve TMV detection efficiency. AuNPs with optimized size and stability were synthesized and introduced into the PCR system. Reaction conditions, including AuNP concentration and thermal cycling parameters, were systematically optimized. A complementary AuNP-based colorimetric assay was also applied to enable visual readout of amplified products. The optimized nanoPCR assay demonstrated improved sensitivity compared to conventional PCR, lowering the detection limit for TMV detection in leaf samples collected in Cao Bằng, Việt Nam. The assay reduced nonspecific amplification and improved reaction reliability. Furthermore, the colorimetric AuNP assay also provided a rapid and equipment-free visualization method, suitable for resource-limited settings. The integration of AuNPs into PCR significantly enhances the detection performance of TMV, while the colorimetric readout provides a simple, field-deployable diagnostic tool. This nanoPCR-based strategy offers great potential for plant virus diagnostics and can be extended to other agriculturally important pathogens.

Keywords: *NanoPCR, gold nanoparticles, Tobacco mosaic virus, Việt Nam, plant virus diagnostics*

PP-18 Application of manganese dioxide nanosheets as an oxidase-mimetic nanozyme for colorimetric detection

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Abstract: Manganese dioxide (MnO₂) nanozymes demonstrate exceptional oxidase-mimetic activity, enabling colorimetric detection of a wide range of biological and chemical analytes via catalytic oxidation reactions. These nanozymes catalyze chromogenic substrates such as 3,3',5,5'-tetramethylbenzidine (TMB), eliminating the need for unstable oxidants and generating distinct visual signals suitable for rapid, on-site screening. The resulting color changes are easily observable by the naked eye or quantifiable using smartphone-based platforms. Advanced heterophase nanostructures further enhance catalytic performance through interfacial charge transfer, while tunable surface properties provide high selectivity against interfering species. With demonstrated applications in small-molecule detection (e.g., paracetamol, ascorbic acid), MnO₂ nanozymes offer a versatile and cost-effective platform that combines simplicity, robustness, and compatibility with complex real samples.

Keywords: *Nanozymes, colorimetric assays, MnO₂, small-molecule detection*

PP-19 Antibacterial and Photothermal Macroporous Ag/HA Composites for Enhanced Solar Steam Generation

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Abstract: Ag/HA nanocomposites with enhanced antibacterial and photothermal properties were successfully developed for solar steam generation. The Ag/HA membrane exhibited strong antibacterial activity against *E. coli* (inhibition zone of 15.5 mm) and *S. aureus* (inhibition zone of 9.5 mm) at a concentration of 28 ppm. The silver incorporation and macroporous structure significantly improved light absorption and water transport, resulting in a high evaporation rate of 1.202 kgm⁻²h⁻¹. These results highlight the potential of Ag/HA as a solution to prevent membrane contamination in solar steam generators.

Keywords: Ag/HA, *Escherichia coli*, *Staphylococcus aureus*, antibacterial activity, solar steam generation.

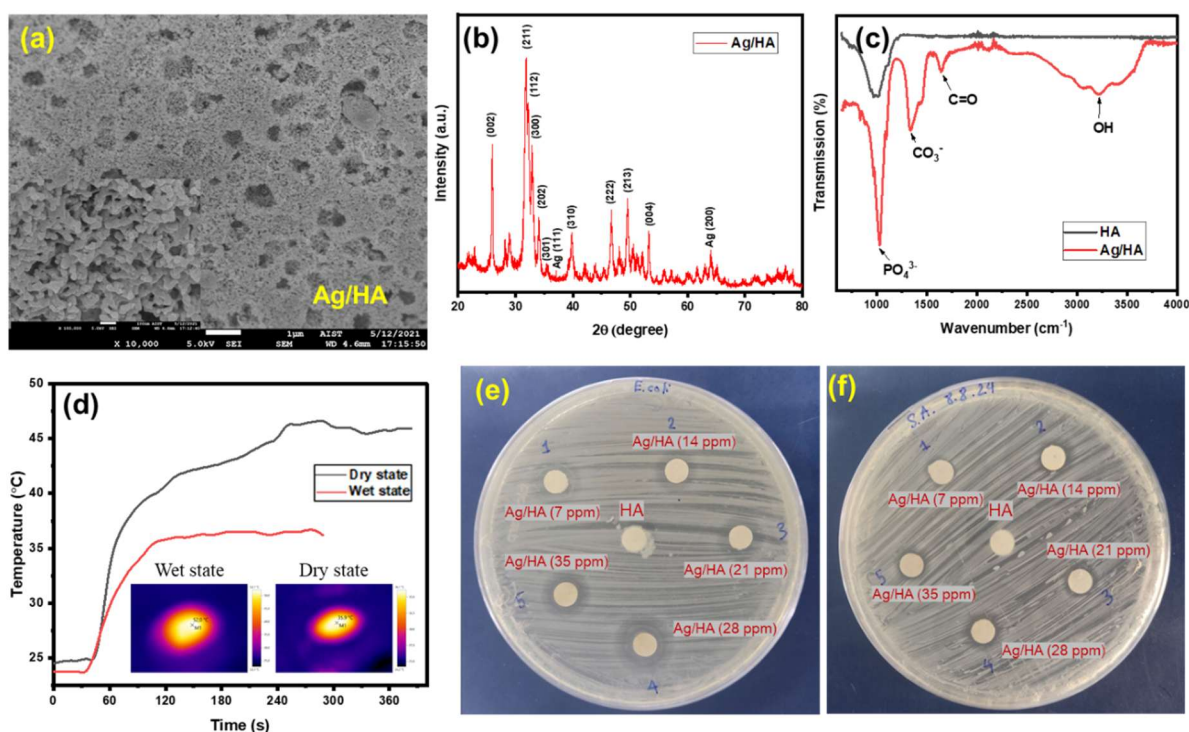


Figure 1: (a) SEM, (b) XRD, (c) FT-IR, (d) the changes in surface temperature of Ag/HA in the wet and dry states and (e, f) Digital images of antibacterial activity for control Ag/HA toward *E. coli* and *S. aureus*

PP-20 **n-SnO₂/n-MoO₃ Nanowires with Enhanced NO₂ Sensing Properties: A Junction-Tuned Approach**

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Abstract: In this work, MoO₃ nanoparticles were coated on SnO₂ nanowires using a sputtering approach with varied sputtering periods (5, 10, and 20 nm). The effect of the MoO₃ sputtering period on the sensors' NO₂ detecting characteristics was investigated. As compared to the other samples, the gas response of the n-SnO₂/n-MoO₃ sensor showed the best efficiency at the optimal time of 5 nm. Our findings indicate that the n-SnO₂/n-MoO₃ heterogeneous sensor is appropriate for real NO₂ gas detection.

Keywords: *SnO₂ nanowires, n-SnO₂/n-MoO₃ heterojunctions, NO₂ sensors*

PP-21 Research the process of synthesizing photocatalytic materials from waste PET plastic to treat polystyrene (PS) microplastics in polluted water

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Abstract: Plastic waste pollution has emerged as one of the most pressing global environmental challenges, with Earth Day 2024 highlighting the theme Planet vs. Plastics and calling for a 60% reduction in plastic consumption by 2040. Among various plastics, polyethylene terephthalate (PET) is widely used and relatively easy to recycle, whereas polystyrene (PS) is both hazardous and difficult to process. In this study, we propose a sustainable strategy that integrates plastic recycling with advanced photocatalysis by converting waste PET into terephthalic acid (TPA), a precursor for synthesizing UiO-66 metal–organic frameworks (MOFs). UiO-66 was further combined with nitrogen-doped TiO₂ (N-TiO₂) to form a N-TiO₂@UiO-66 composite. Structural and morphological analyses by XRD and SEM confirmed the successful formation of the composite, where N-TiO₂ nanoparticles were uniformly dispersed on UiO-66 surfaces. Optical characterizations demonstrated enhanced charge separation efficiency and reduced band gap energy (1.74 eV), suggesting superior photocatalytic activity. The photocatalytic performance was evaluated for PS degradation in both thin-film and aqueous systems. Results indicated that PS–(N-TiO₂@UiO-66) composite films achieved 36% weight loss after 9 weeks under visible light irradiation, while PS degradation in aqueous solution reached up to 98% within 30 h. FT-IR spectra confirmed the disappearance of characteristic PS peaks and the appearance of intermediate products, indicating effective photodecomposition. This work not only addresses plastic waste management by valorizing PET but also provides an efficient photocatalytic pathway for eliminating hazardous PS microplastics in water, contributing to environmental protection and sustainable development.

Keywords: Microplastic, photocatalyst, PS treatment, N-TiO₂@UiO-66, environment

PP-22 Green chemistry approach for silver nanoparticle synthesis from medicinal plants: Antimicrobial efficacy and practical applications

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Abstract: The uncontrolled growth of microorganisms poses significant threats to food safety and human health, while the overuse of antibiotics has accelerated the emergence of resistant strains. Silver nanoparticles (AgNPs) have been recognized as effective broad-spectrum antimicrobial agents, and green synthesis using plant extracts offers an eco-friendly alternative to conventional methods. In this study, aqueous extracts of *Elsholtzia cristata* (Vietnamese balm) and *Cymbopogon citratus* (lemongrass) were employed as reducing and stabilizing agents for the green synthesis of AgNPs. The synthesized nanoparticles were characterized by UV–Vis spectroscopy, TEM, and FT–IR. UV–Vis analysis confirmed optimal synthesis at 3 h with 10 mL of plant extract and an AgNO₃:PVA mass ratio of 1:1. TEM revealed spherical nanoparticles with average sizes of ~9 nm for *E. cristata*-mediated AgNPs and ~20.7 nm for *C. citratus*-mediated AgNPs, both with narrow size distributions and minimal aggregation due to a natural biocapping layer. FT–IR spectra indicated the involvement of phenols, alcohols, and flavonoids in nanoparticle reduction and stabilization. Antimicrobial assays demonstrated strong inhibitory effects of AgNPs against *Escherichia coli* and *Staphylococcus aureus*, as well as antifungal activity against *Candida albicans*. Furthermore, AgNPs enhanced the preservation of agricultural products such as grapes and tomatoes for up to 21 days, and AgNP-impregnated gauze exhibited high antibacterial efficacy. These findings highlight that green synthesis using local plant extracts is a simple, cost-effective, and environmentally friendly method for producing stable AgNPs with potent antimicrobial activity. The synthesized AgNPs show great potential for applications in agriculture, healthcare products, and biomedical materials.

Keywords: *Cymbopogon citratus*, Silver nanoparticles (AgNPs), Green synthesis, Antibacterial, AgNP-impregnated gauze

PP-23 Encapsulation of Apigenin into Chitosan Nanoparticles to Enhance Solubility, Stability, and Pharmacological Potential

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Abstract: Apigenin, a plant-derived flavonoid, is well recognized for its antiviral, anti-inflammatory, and antioxidant activities. However, its poor solubility significantly limits its bioavailability. In this study, apigenin was encapsulated within a chitosan–sodium tripolyphosphate (TPP) crosslinked network and subsequently processed by probe sonication to enhance dispersion and formulation stability. Reaction parameters, including time, stirring speed, concentrations, and component ratios, were optimized to obtain nanoparticles with small, uniform, and stable sizes. The resulting apigenin/chitosan nanoparticles exhibited an average hydrodynamic diameter of 171 nm, with solubility increased by more than 38-fold compared to pure apigenin (0.0013 → 0.05 mg/mL). Characterization analyses using UV–Vis and FTIR spectroscopy demonstrated spectral shifts corresponding to structural modifications of apigenin upon encapsulation. The marked improvement in apigenin dispersibility highlights its potential to maximize diverse pharmacological effects, particularly in the treatment of inflammatory and viral diseases

Keywords: *apigenin; chitosan nanoparticles; bioavailability; encapsulation; antiviral and anti-inflammatory activity*

PP-24 Enhancement of Torsional Vibration Resonances in AFM Microcantilevers Using a Transition Section

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Abstract: Torsional modes of atomic force microscope (AFM) cantilevers have been widely used to probe lateral interactions between biomolecules and to study cell membranes, proteins, and DNA under mechanical stress, offering exceptional sensitivity and versatility across diverse environments (air, water, and liquid). Recent research, however, has increasingly focused on improving imaging resolution and measurement sensitivity by tailoring cantilever geometry. In this study, we enhance torsional sensitivity by introducing a transition region into the cantilever, which leads to variations in the resonant frequency. Our results reveal the emergence of multiple spatial maxima in higher-order modes and demonstrate how the structure of transition section enables tunable frequency shifts. In addition, we propose a sensitivity function that quantifies the dependence of the modal response on tip–surface coupling stiffness, uncovering nontrivial geometry-dependent trends. These findings establish clear design principles for enhancing AFM sensitivity through geometric control and provide a robust theoretical framework for optimizing next generation microcantilever probes to meet demanding operational requirements.

Keywords: Torsional sensitivity, AFM microcantilever, Modal sensitivity, Euler- Bernoulli beam theory, Analytical method.

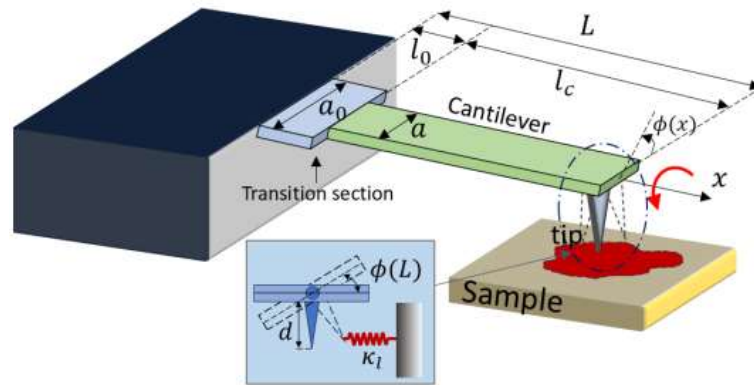


Figure: A cantilever beam with a transition region of length l_0 and width a_0 is also fixed to the base at $x = 0$ (black region). For $a_0 > a$, the structure forms an overhang-shaped cantilever. The torsional oscillations are analyzed with respect to the sample through the effective interaction stiffness κ_t (inset).

PP-25 Effect of some technological factors in the process of jam from pineapple added coconut cream

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Abstract: Pineapple (*Ananas comosus*) is a nutritious tropical fruit often eaten as fresh or processed products such as pineapple juice, concentrated pineapple juice, and dried pineapple... Currently, pineapple puree products are not popular on the market, and there has still not been complete research on the processing technology of this product. This study aimed to determine some technological parameters, including coconut milk mixing ratio, additional citric acid content, additional pectin content, added sugar ratio, and appropriate concentration time to create products with the best sensory quality in terms of structure, color, smell, and taste. Factors include total soluble solids content (TSS) (pre-concentrate and post-concentrate), pH (pre-concentrate and post-concentrate), total organic acid content, and sensory evaluation were monitored in each experiment. According to the results, the ratio of mixing coconut cream (80/20), the content of added citric acid (0.4%), the added pectin content (0.7%), the ratio of added sugar (85/15), and the concentration time (30 minutes) are suitable for processing this product with the best sensory quality.

Keywords: *Pineapple (Ananas comosus), coconut cream, acid citric, pectin, sugar, concentration-time*

PP-26 Genetic Diversity Evaluation of some Honeysuckle Species Commonly Used as a Traditional Medicine in Vietnam

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Abstract: Honeysuckle has been used for thousands of years as a traditional medicine to treat many different diseases. In Vietnam, 11 *Lonicera* species are distributed naturally from the North to the Central Highlands. *L. japonica*, *L. confusa*, and *L. macrantha* are commonly used as traditional medicine in Vietnam. In this study, a total of 20 samples of 3 honeysuckle species collected in Vietnam were evaluated for genetic diversity using ISSR markers. Using 10 selective primers produced an average of 8.5 loci/primer, the polymorphism rate was 85.53%. The highest difference between primer pairs (Rp) was 6.4 (primer U824), the lowest was 2.6 (primer U815) and the average Rp index was 3.83. The mean PIC coefficient was 0.32, ranging from 0.26 to 0.40, indicating that the study's polymorphism level was high. The mean genetic similarity coefficient was 0.68, ranging from 0.48 to 0.99. A total of 20 samples were divided into 3 main clusters: group I (*L. confusa*), group II (*L. macrantha*), and group III (*L. japonica*). The present study results are useful for the conservation and breeding of honeysuckle varieties.

PP-27 Synthesis of SiO₂/chitosan-based composite scaffolds and assessment of their bioactivity for potential use in bone tissue engineering

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Abstract: Bone tissue engineering (BTE) is an effective method for bone repair and regeneration, with many advantages over traditional bone grafting methods. Silica (SiO₂) is renowned for its exceptional properties, including bioactivity, biocompatibility, and non-cytotoxicity. In addition, silica also exhibits a high affinity for HAp, which is known to be the main inorganic component of bone structure, thereby supporting cell adhesion and proliferation. With these advantages, silica is a good candidate for biomedical material synthesis.

This work presents the synthesis and characterization of three-dimensional (3D) chitosan/silica (CS/SiO₂) scaffolds prepared by the freeze-drying method for bone tissue engineering applications. The morphology and structural features of the scaffolds were investigated by scanning electron microscopy (SEM) and liquid substitution techniques. The CS/SiO₂ scaffolds exhibited highly porous and interconnected structures with rough surfaces and thick pore walls, exceeding 100 µm. The average pore size was 303 ± 56 µm, while the porosity values were 72.38% in water and 33.95% in ethanol. These pore characteristics are suitable for facilitating cell attachment, nutrient transport, and tissue ingrowth. The incorporation of SiO₂ nanoparticles into the chitosan matrix improved the scaffold's structural stability and provided potential sites for enhanced bioactivity. The obtained results suggest that the freeze-dried CS/SiO₂ scaffolds possess a favorable pore architecture and physical properties, making them promising candidates for bone tissue engineering.

Keywords: *Bone tissue engineering, Bioactivity, Scaffold, Chitosan, Silica.*

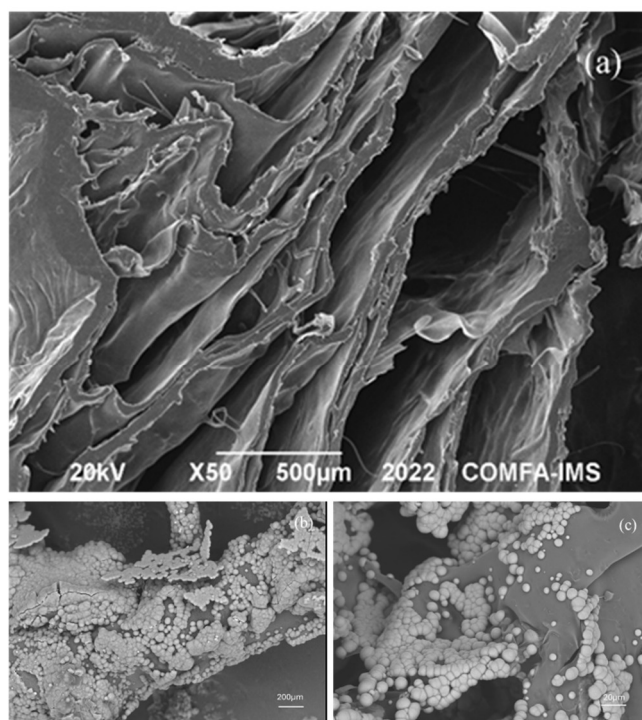


Figure: (a) Microstructured HAp/CS scaffold; (b) Biomineral layer formed on the surface of the scaffold on day 7; (c) Biomineral layer formed on the surface of the scaffold on day 14

PP-28 Molecular Dynamics Simulations for the Selection of a Lipopolysaccharide Binding Aptamer Characterized by Electrochemical Analysis

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Abstract: Lipopolysaccharides (LPS), key components of the outer membrane of Gram-negative bacteria, play a crucial role in bacterial pathogenicity and can trigger severe immune responses, leading to sepsis, endotoxic shock, and other inflammatory diseases. Rapid and accurate LPS detection is essential for diagnosing bacterial infections, monitoring pyrogenic contamination in pharmaceuticals, and ensuring food safety. Aptamer-based detection offers a promising alternative to traditional methods, providing enhanced sensitivity, specificity, and cost-effectiveness. Recent advances in molecular simulations have further improved aptamer selection by complementing the conventional Systematic In this study, we combined conventional aptamer selection with computational studies to generate a single-stranded DNA (ssDNA) aptamer with high affinity and selectivity for LPS detection. After 10 rounds of SELEX, the obtained sequences were subjected to docking analysis. Based on the docking outcome, three sequences including aptamer Seq 5, Seq 7, and Seq 9 were selected for further evaluation of their affinity to LPS by both experimental assays and molecular dynamics simulation. The results of both experimental and simulation methods indicated that aptamer Seq 5 showed the best affinity to LPS of *Klebsiella Pneumonia* ATCC 15380.

PP-29 Development of pH-Sensitive Redox Nanoparticles for Stomach Protection in Aspirin-Induced Gastric Ulcer Mouse Model

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Abstract: Gastric ulcer (GU) which is a common gastrointestinal disease, has affected millions of lives. While its etiology remains unclear, overproduction of reactive oxygen species (ROS) has been considered as the primary driving mechanism. A variety of low-molecular-weight antioxidants have been utilized in the prevention of GU; however, these conventional treatments are not uniformly successful due to their systemic distribution, resulting in adverse side effects and disruption of intracellular redox equilibrium. This research presents two distinct self-assembling micellar nanoparticles (RNPs) with a TEMPO moiety (a ROS scavenger), each measuring several tens of nanometers, developed for oral protection of GU. One of them, termed RNP^N, decomposes at acidic pH, whilst the other, identified as RNP^O, maintains stability regardless of pH fluctuations. Both kinds of RNPs demonstrated unique free radical scavenging capabilities *in vitro*. RNP^N exhibits significant improvement in antioxidant activity when pH decreases, due to the protonation of amino linkages in its side chains, resulting in the collapse of the micellar structure and the exposure of the TEMPO moieties on the core to the external environment. In contrast, RNP^O with ether linkages in the side chains maintained its spherical structure, resulting in sustained antioxidant activity regardless of pH fluctuations. Orally administered RNP^N demonstrated enhanced *in vivo* gastric accumulation and retention relative to RNP^O, due to the interactions between the protonated positively charged segments of RNP^N and the negatively charged surface of the gastric epithelium in acidic circumstances. RNP^N demonstrated superior protection against oxidative stress induced by aspirin in the GU mouse model, due to its increased gastric accumulation and retention, as well as its higher capacity for reactive oxygen species scavenging in acidic pH conditions, relative to RNP^O (**Figure 1**). Moreover, both RNPs exhibit negligible toxicity to murine macrophages and zebrafish embryos, signifying their biosafety. Thus, RNPs, particularly RNP^N, may function as a potential nanotherapeutic for the oral prevention of GU.

Keywords: reactive oxygen species, oral delivery, pH-sensitive, redox nanoparticles, aspirin-induced gastric ulcer.

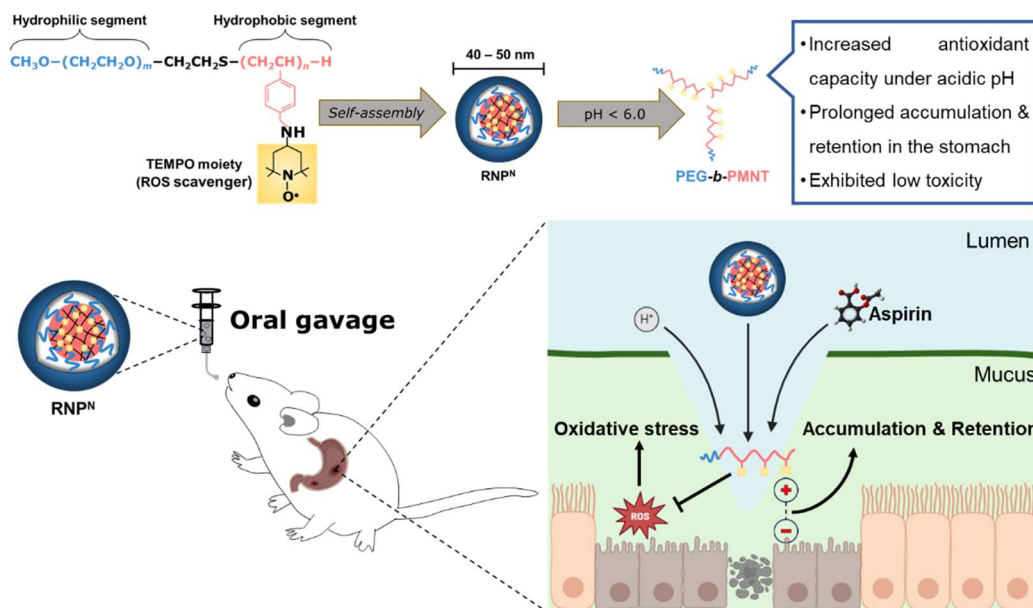


Figure 1: The structural illustration of RNP^N and its protective effects in aspirin-induced GU model.

References:

Tang, M. D. Q., Tran, N. B., Nguyen, T. H. T., Nguyen, K. U. H., Trinh, N. T., Van Vo, T., ... & Vong, L. B. (2024). Development of oral pH-sensitive redox nanotherapeutics for gastric ulcer therapy. *Journal of Controlled Release*, 375, 758-766.

PP-30 Luminescent carbon quantum dots via green microplasma synthesis from orange juice

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Abstract: Carbon quantum dots (CQDs) have emerged as a highly promising class of nanomaterials due to their unique optical, chemical, and electrical properties. Their appeal lies in their exceptional chemical and physical stability, biocompatibility, and environmental friendliness, which distinguish them from traditional metal-semiconductor quantum dots that often suffer from toxicity issues. Among their most notable features are their tunable luminescent properties, which make them ideal for applications such as bioimaging, light-emitting devices, and sensing.

The synthesis of carbon quantum dots (CQDs) has been achieved through multiple methods, each with distinct advantages and limitations. Among these, microplasma processing offers several key benefits, including rapid synthesis, uniform particle size distribution, and precise control over particle size and physicochemical properties.

In this study, we adopted a hybrid strategy combining both “top–down” and “bottom–up” approaches by utilizing orange juice as a natural and sustainable carbon source. This choice not only simplifies the synthesis process but also aligns with the increasing demand for environmentally friendly and cost-effective methods.

PP-31 β -Cyclodextrin-Based Polymeric Nanocarriers for α -Mangosteen Delivery to Inhibit HeLa Cell Proliferation

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Abstract: Cyclodextrin-based polymeric nanoparticles (β -CDNP), developed by Prof. Sakurai's group (Kitakyushu University, Japan), provide a promising nanocarrier system for enhancing the solubility, stability, and bioavailability of therapeutic compounds. In this study, α -mangosteen (AMG), a natural xanthone with reported anticancer activity, was encapsulated into β -CDNP and evaluated for its physicochemical properties, release behavior, and cytotoxic effects on HeLa cells. The AMG-CDNP nanocomplex exhibited an average particle size of 132.5 nm and demonstrated a biphasic release profile, with around 50% of AMG released within the first 24 hours followed by sustained release over 96 hours. Cytotoxicity assessment using the MTT assay revealed that AMG-CDNP showed an IC₅₀ of 8.2 μ g/mL after 24 hours, compared to 4.8 μ g/mL for free AMG. However, after 48 hours, the antiproliferative effect of AMG-CDNP was comparable to that of free AMG, indicating the ability of the nanocarrier to prolong the therapeutic impact. These findings suggest that β -CDNP is an effective delivery platform for AMG, enabling controlled release and extended anticancer activity against HeLa cells.

PP-32 Preparation of gold nanoparticles stabilized in water-soluble β -glucan by gamma irradiation with high antioxidant and anticancer activities

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Abstract: Gold nanoparticles (AuNPs) were successfully synthesized by gamma irradiation of $[\text{Au}^{3+}]$ solution with concentration of 0.25–1.5 mM using water-soluble yeast β -glucan as a stabilizer. The UV-vis spectra obtained solutions of AuNPs showed the maximum absorption wavelengths (λ_{max}) at 518–524 nm. Results of the transmission electron microscope (TEM) images revealed that the average particle sizes of AuNPs increased from 5.3 to 17.5 nm with the increase of $[\text{Au}^{3+}]$ concentrations from 0.25 to 1.5 mM, respectively. The crystalline structure of the AuNPs was also validated through X-ray diffraction (XRD) analysis. The interaction of β -glucan with AuNPs via steric coordination linkages ($-\text{Au}\dots\text{O}-$) was identified through Fourier transform infrared (FTIR) spectroscopy. The antioxidant activity of AuNPs investigated using free radical ABTS[•] indicated that this activity was strongly dependent on the concentration and size of AuNPs. In addition, the MTT (3[4,5 dimethylthiazol-2-yl]-2,5-diphenyltetrazol bromide) assay performed on a liver cancer cell line (HepG2) distinctly demonstrated that the treatment of 0.1 mM AuNPs strongly inhibited the growth of HepG2 cells. Meanwhile, the growth of the fibroblast cell line (L929) was almost unaffected by the same treated concentrations of AuNPs. Thus, due to the high purity, biocompatibility, and high anticancer and antioxidant activity of AuNPs synthesized by the γ -ray irradiation method, this prepared AuNPs/ β -glucan can potentially be used as an antioxidant and an anticancer agent.

Keywords: Anticancer, antioxidant, β -glucan, HepG2, gold nanoparticles, γ -ray irradiation

PP-33 Fabrication of Fluorescent PDMS/RhB Microspheres for Antibody Purification Applications

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Abstract: Optical microscopy was employed to record fluorescence intensity changes of PDMS microspheres encapsulating Rhodamine B (PDMS/RhB) during successive surface molecular conjugations, providing a basis for detecting botulinum antibodies in protein extract samples. In this study, the microspheres were synthesized using a microfluidic technique, yielding stable spherical particles with an average diameter of ~200 μm and exhibiting bright fluorescent properties suitable for optical detection. Observation under a fluorescence microscope at 560 nm excitation, combined with automated image processing, revealed a correlation between particle size and fluorescence intensity. Following surface functionalization with amine groups (via APTES) and subsequent modification with carboxyl groups (via succinic anhydride), the microspheres were covalently conjugated with the light chain type A (LC/A) antigen of botulinum neurotoxin type A using EDC/NHS coupling chemistry. When incubated with crude protein extracts containing nanobody antibodies specific to LC/A along with non-target proteins, a change in fluorescence intensity was observed, suggesting selective antibody binding. The variation in fluorescence intensity of the microspheres at different dilutions of the protein extracts demonstrates their potential for fluorescence-based purification and quantification. This study highlights the applicability of PDMS/RhB microspheres as a simple and efficient optical tool for detecting LC/A-specific antibodies in complex biological environments.

Keywords: *Microspheres, PDMS, Microfluidic, Biosensor, Botulinum type A.*

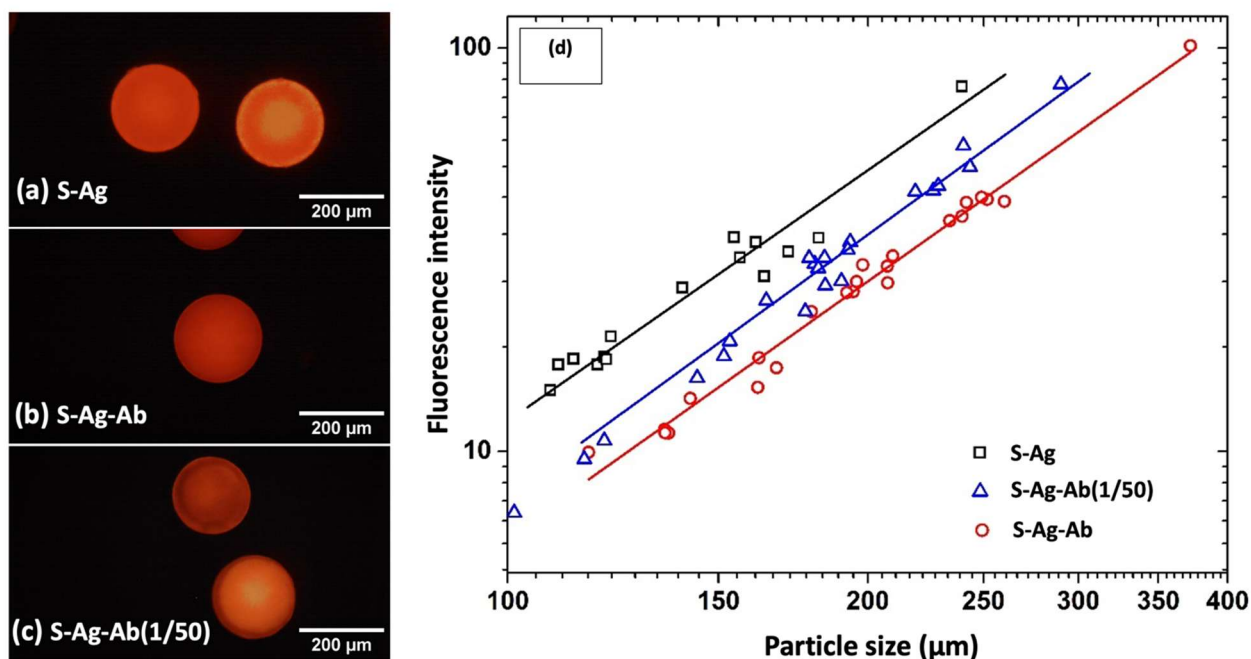


Figure: Representative fluorescence images of PDMS/RhB microspheres upon antibody binding at different concentrations. (a) PDMS/RhB microspheres with immobilized antigen; (b) PDMS/RhB microspheres with antigen incubated with undiluted antibodies; (c) PDMS/RhB microspheres with antigen incubated with antibodies diluted 50-fold; (d) Fluorescence intensity as a function of particle size for antigen-conjugated PDMS/RhB microspheres with and without antibody binding.

PP-34 Study on the fabrication of nanobody conjugated amine-magnetic particles for the purification of botulinum toxin type A light chain

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Abstract: Botulinum neurotoxin type A is one of the most potent protein toxins known, with its light chain (Lc/A) acting as the principal effector that blocks neurotransmission. Consequently, Lc/A has emerged as a critical target for mechanistic studies, inhibitor development, and diagnostic tool design. In this study, we developed an affinity system based on Fe₃O₄@SiO₂-NH₂ magnetic beads conjugated with the nanobody A8 - a small, high-affinity antibody-like protein that selectively recognizes Lc/A. This platform facilitates the purification and enrichment of Lc/A from complex protein mixtures and dilute solutions. Quantitative assessment revealed that 0.3 mg of the functionalized beads could immobilize approximately 18 µg of A8, corresponding to an immobilization efficiency of around 90%, thereby enabling the effective capture of approximately 9.5 µg of Lc/A. Following magnetic separation, the concentration of Lc/A in the resultant solutions was enriched twelvefold. These results demonstrate that nanobody-conjugated amine functionalized magnetic particles constitute a promising approach for the detection and analysis of Lc/A, especially in complex matrices or low-abundance contexts such as food safety testing and clinical diagnostics.

Keywords: Botulinum neurotoxin type A (BoNT/A), nanobody A8, magnetic nanoparticles, protein purification, enrichment, immunoprecipitation

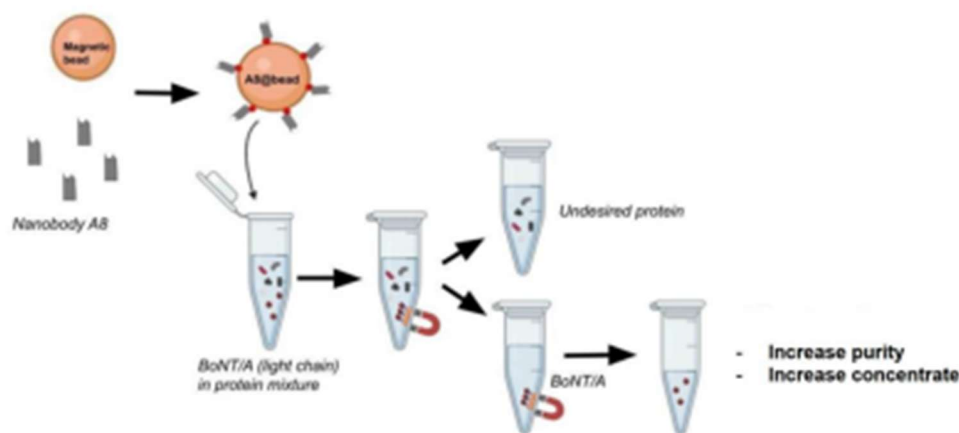


Figure: Diagram of immunoprecipitation process

PP-35 Temperature-modulated toxicity of bisphenol A in zebrafish (*Danio rerio*) embryos: morphological, physiological, and transgenerational responses

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Abstract: Bisphenol A (BPA), a widely used plastic additive compound and known as an endocrine disruptor, is frequently detected in aquatic environments. Temperature, an important climate stressor, can influence pollutant toxicity, but the combined and transgenerational effects of BPA under different temperatures remain poorly understood. This study used zebrafish embryos (*Danio rerio*) to evaluate developmental and biochemical responses to BPA exposure (0–5 mg/L) under three temperatures (23°C, 28°C, 33°C) across two generations (F0 and F1). Endpoints included mortality, morphological malformations, hatching rate, heartbeat, and glutathione-S-transferase (GST) activity as physiological stress markers. Results showed that BPA exposure induced dose-dependent increases in mortality and malformations, and delayed hatching in both generations. High temperature (33°C) exacerbated BPA toxicity, resulting in higher mortality, increased malformations, delayed hatching, elevated GST activity, and reduced heartbeat in F0 and F1 embryos. In contrast, low temperature (23°C) delayed development and reduced hatching success. F1 embryos were more sensitive than F0, showing greater mortality, malformations, and GST activity in the 5 mg/L BPA + 33°C treatment, indicating potential transgenerational effects. These findings demonstrate that BPA-induced developmental toxicity in zebrafish is strongly modulated by environmental temperature, affecting survival, morphogenesis, and physiological stress responses across generations. The study underscores the importance of incorporating climate-related stressors into ecological risk assessments of endocrine-disrupting chemicals.

Keywords: Bisphenol A (BPA), zebrafish embryos, temperature stress, Glutathione-S-transferase (GST) activity

PP-36 Non-invasive prediction of colorectal cancer using an ensemble stacking model based on circulating mRNA

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Abstract: Colorectal cancer (CRC) is a leading cause of cancer-related death worldwide. Current invasive diagnostic methods for CRC often cause psychological distress in patients, limiting their applicability in screening programs. This study aims to identify novel non-invasive blood-based biomarkers for CRC screening by analyzing gene expression data. Whole blood mRNA microarray datasets, including E-MTAB-1532 (n=200), E-MEXP-3756 (n=60), GSE164191 (n=121), and GSE10715 (n=30), were retrieved from two public repositories ArrayExpress and the Gene Expression Omnibus (GEO). Following data normalization, we performed differential gene expressions (DEGs) and ROC curve analyses and identified forty-seven candidate genes through Venn diagram analysis. The prediction model was built using the top five genes, *SORT1*, *ECHDC3*, *LBH*, *TRAC*, and *TGFBR3*, identified by the feature selection method. Three datasets, E-MTAB-1532, E-MEXP-3756, and GSE164191, were combined and split into training and testing sets (70:30 ratio), using GSE10715 as an independent validation cohort. The model was built based on the ensemble stacking techniques, incorporating base learners including Random Forest, k-Nearest Neighbors, Support Vector Machine, Heteroscedastic Discriminant Analysis, bagEarth, AdaBoost, Gradient Boosting Machine, Earth, Generalized Additive Model, and Flexible Discriminant Analysis, with Neural Network used as the meta-learner to combine their outputs. This model demonstrated promising performance with an AUC of 0.824 on the testing set and 0.928 on the validation set. These findings suggest that the established five-gene model holds significant potential as a novel, non-invasive blood-based tool to support the screening of individuals at risk of colorectal cancer.

Keywords: *Colorectal cancer, machine learning, blood-based biomarker, microarray*

PP-37 Toward enhanced bioavailability and controlled release of poorly soluble drugs by room-temperature atomic layer deposition: a case study of gliclazide

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Abstract: Poor aqueous solubility is a major challenge in drug formulation, often limiting the bioavailability and therapeutic efficacy of many pharmaceutical compounds. Traditional strategies, such as amorphous solid dispersions, lipid-based formulations, and cyclodextrin complexation, have been widely used to improve drug solubility. However, these approaches often suffer from stability issues, drug-excipient incompatibility, and complex manufacturing processes. In this study, we explore the application of atomic layer deposition (ALD) as a surface engineering technique to improve the dispersion of poorly soluble drugs, demonstrated for gliclazide – a sulfonylurea antidiabetic drug used to treat type 2 diabetes mellitus. By coating GLZ particles with ultra-thin SiO₂ films, their wettability is remarkably improved, promoting a highly dispersed state in aqueous medium and significantly accelerating the dissolution. More importantly, by controlling the number of ALD cycles, the release rate of GLZ can be tailored, enabling tunable drug dissolution profiles. At lower ALD cycles, dissolution is enhanced due to improved dispersion, whereas at higher cycle numbers, the coating forms a diffusion barrier, regulating drug

release. This key achievement demonstrates the potential of SiO₂ ALD not only in overcoming solubility-related limitations but also in providing a method of multi-purpose design for controlled drug delivery. Given its compatibility with pharmaceutical manufacturing, ALD presents a promising pathway to enhance bioavailability and optimize release kinetics of poorly soluble drugs.

Keywords. Poorly water-soluble drugs, controlled release, SiO₂ coating, bioavailability, atomic layer deposition, fluidized bed reactor, room-temperature coating, gliclazide.

PP-38 Stable dispersion and prolonged dissolution of hydrophilic pharmaceutical achieved by room-temperature atmospheric pressure atomic layer deposition

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Diclofenac sodium (DCF), a common non-steroidal anti-inflammatory drug (NSAID), has been widely used in clinical context as tablet and capsule, but demonstrates sedimentation in water and poses challenges to liquid dosage forms. In this study, atomic layer deposition (ALD) was employed in order to modify its characteristics. The technique was performed at room temperature, using a home-built fluidized bed reactor, with silicon tetrachloride and distilled water as precursor and co-reactant, respectively. By sequential introduction of precursor and co-reactant to the reacting chamber, a coating layer on the surface of metformin hydrochloride powder was generated. While the XPS result revealed that SiO₂ was the major constituents of the coating layers, Fourier transform infrared spectroscopy (FTIR) and X-ray diffraction (XRD) experiments confirmed no change in the structure of the initial material, which is predicted to maintain its pharmacological effects. Further measurement reveals that ALD coating has increased the intensity of zeta potential to above 30 mV – the value that ensures substantial repulsive interaction among particles. This enhancement remarkably improved the dispersibility of DCF powder, reflected by the variation in relative illuminance of corresponding suspension. In addition, as the number of ALD cycles increased, the thicker coating layer was obtained, and this contributed to a remarkably delayed *in vitro* release. Specifically, applying 25 ALD cycles slowed down the release rate by 1.5 times, whereas the value was increased to 2.3 times with 50 ALD cycles. This result opens up the potential for creating not only an extend-release but also suspension dosage form for diclofenac sodium.

PP-39 Molecular Dynamic Simulation Study of Deformation Behavior and the Role of Chitosan in Reinforcing Bombyx mori Fibroin Composites Under Acidic Conditions

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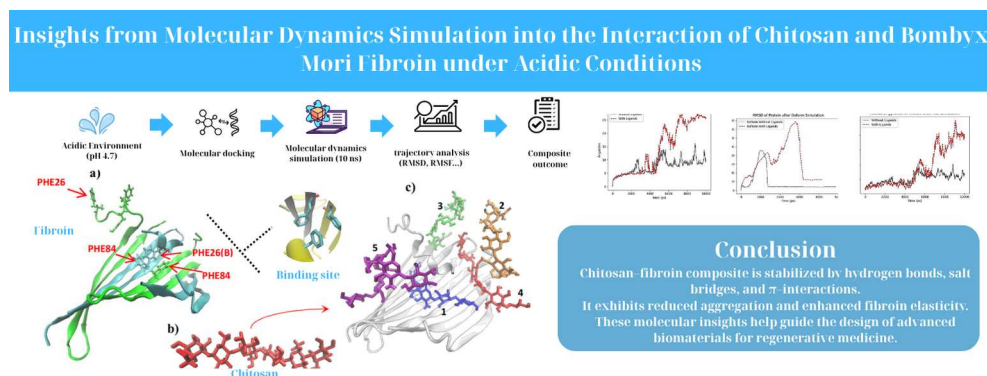
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Abstract: Despite the demonstrated potential of fibroin and chitosan composites, the precise molecular mechanisms behind their interactions, particularly the interplay between fibroin's hierarchical assembly and chitosan, remain unclear. We employed molecular docking and molecular dynamics simulations to investigate the structure and interactions between chitosan and fibroin. Detailed trajectory analyses, including evaluations of root mean square deviation (RMSD), root mean square fluctuation (RMSF), radius of gyration, and deformation metrics, were conducted to reveal the underlying molecular determinants that govern composite formation. The investigated mechanical properties of the chitosan-fibroin complex reveal potential advantages. The complex exhibits reduced aggregation tendencies, as indicated by greater fluctuations in the radius of gyration and enhanced fibroin elasticity. By using methodologies from computational physics and materials science, our study aims to bridge the gap between experimental observations and molecular-scale interactions, ultimately guiding the development of advanced fibroin-based composites. These insights hold the promise of informing the design of novel biomaterials with enhanced mechanical, biological, and physicochemical properties, in line with the current thrust toward personalized and regenerative medicine.

Keywords: biomaterial, polymer, drug delivery, molecular dynamic simulation, chitosan, fibroin.

Graphic Abstract



PP-40 Density Functional Theory Perspective On Single – Atom Fe/N-Embedded Graphdiyne As An Efficient Electrocatalysts For The Hydrogen Evolution Reaction

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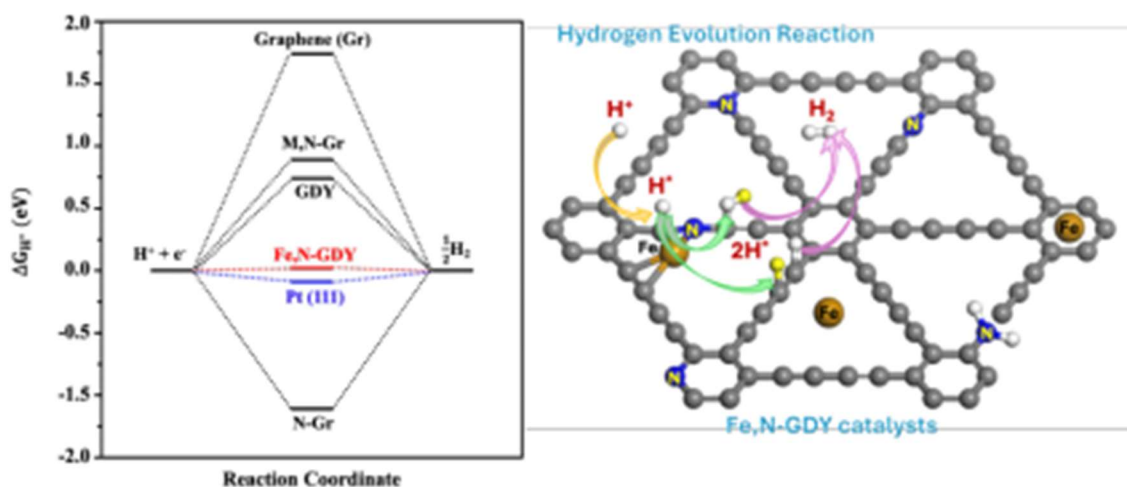
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Abstract: The development of stable, efficient, and cost-effective electrocatalysts for the hydrogen evolution reaction (HER) is crucial for advancing sustainable hydrogen production, a key component in achieving clean energy goals and reducing reliance on fossil fuels. Recent theoretical and experimental studies have highlighted the promising performance of M-N-C (Metal-Nitrogen–Carbon) based carbon allotropes as HER electrocatalysts. In this study, we perform a comprehensive density functional theory (DFT) investigation of graphdiyne (GDY) co-doped with iron (Fe) and nitrogen (N), namely Fe,N-GDY aiming to assess its catalytic potential for HER. Our calculations reveal that Fe,N-functionalized GDY exhibits improved structural stability, enhanced electrical conduct, and a narrowed bandgap relative to pristine GDY. The hydrogen adsorption sites on Fe,N-GDY were systematically analyzed, with hydrogen adsorption free energy (ΔG_{H^*}) values approaching zero, specifically 0.020 eV for the H3@Fe, N3-GDY model, closely aligning with the performance benchmark of Pt(111) (– 0.090 eV). These findings suggest that Fe,N-GDY is a compelling candidate for HER catalysis and offer valuable insights for the rational design of carbon-based single-atom catalysts for green hydrogen production.

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Keywords: Graphdiyne, Electrocatalyst, Iron-Nitrogen codoped Grapdiyne, Hydrogen Evolution Reaction.



PP-41 Access to Functionalized α,β -Unsaturated Imines through Bicyclic Ketone Intermediates

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Abstract: α, β -Unsaturated imines are valuable intermediates for the synthesis of bioactive molecules and potential pharmaceutical candidates. Developing efficient synthetic routes to these compounds provides important tools for biomedical research and drug discovery. This study aims to design and establish a multi-step pathway for constructing α, β -unsaturated imines from readily available precursors. The synthetic strategy involved sequential transformations, including a Diels–Alder reaction of 1,3-cyclohexadiene and methyl vinyl ketone, catalytic hydrogenation, Baeyer–Villiger oxidation, PCC-mediated oxidation, and an imine condensation step with 2,6-diisopropylaniline. Grignard additions to aromatic substrates were also explored to expand structural diversity. Key bicyclic ketone intermediates were successfully synthesized, and the imine condensation afforded crystalline imine products in good yield. Parallel reactions delivered additional functionalized intermediates, demonstrating the robustness of the synthetic design. This work establishes a feasible and versatile approach to α, β -unsaturated imines, highlighting their potential as precursors in the synthesis of bioactive compounds and laying the foundation for future biomedical applications.

PP-42 Lipid–Gold nanoparticles–Curcumin Conjugates as Plasmon-Enhanced Antimicrobials Against Multidrug-Resistant *Escherichia coli*

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Abstract: Antibiotic resistance remains one of the most global health threats, driving the demand for innovative antimicrobial strategies. In this study, we report the development of a lipid–gold nanoparticle–curcumin conjugate (Lipid@AuNPs@Cur) designed to improve the solubility and antibacterial activity of curcumin via the surface plasmon resonance (SPR) properties of AuNPs. AuNPs were synthesized using an electrochemical method and subsequently incorporated into a lipid–curcumin matrix. The antibacterial activity of Lipid@AuNPs@Cur was assessed against multidrug-resistant *Escherichia coli* and compared with free saturated curcumin under both dark conditions and 532 nm laser irradiation. Without irradiation, Lipid@AuNPs@Cur demonstrated approximately 30-fold greater antibacterial activity relative to free curcumin. Upon 532 nm laser exposure, a plasmon-assisted photothermal effect further potentiated antibacterial activity, reducing bacterial viability by more than 50% compared to non-irradiated controls. These findings underscore the synergistic contributions of the lipid carrier, AuNP-mediated SPR, and curcumin, resulting in a multifunctional antimicrobial platform. In conclusion, the electrochemically synthesized Lipid@AuNPs@Cur conjugate offers a promising strategy to improve the bioactivity of curcumin while delivering potent antibacterial activity against multidrug-resistant *E. coli*. This nanostructured system highlights the potential of integrating phytochemicals with nanomaterials and photothermal activation to advance the next generation of antimicrobial therapeutics.

Keywords: lipid carrier; gold nanoparticles; curcumin; antibacterial activity; photothermal effect

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