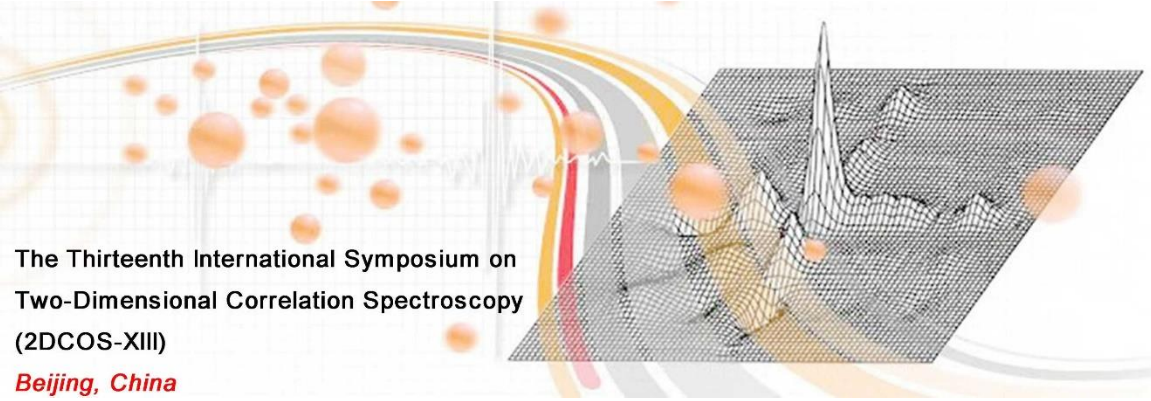
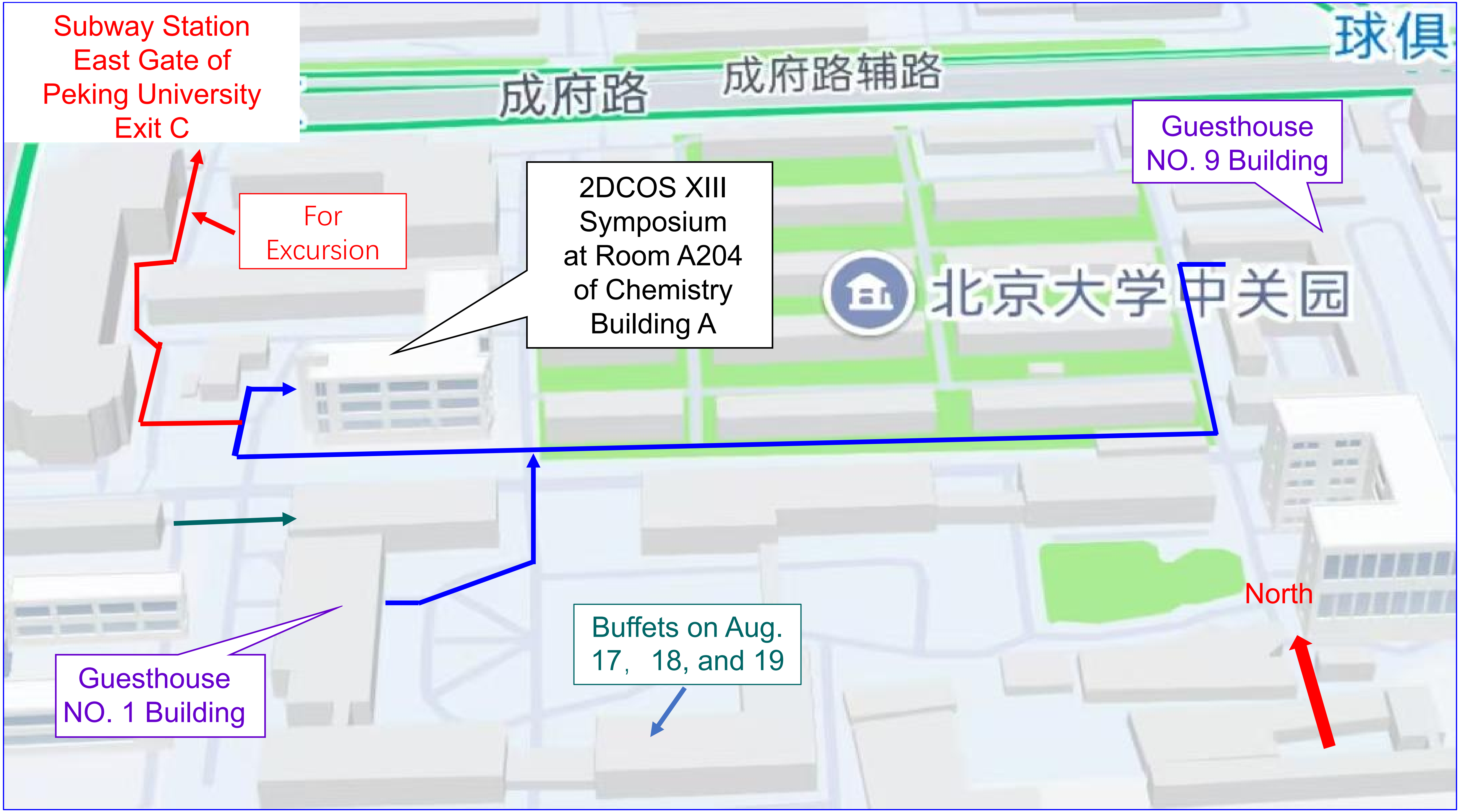


2DCOS-XIII

The Thirteenth International Symposium on Two-Dimensional Correlation Spectroscopy

August 16 - 19, 2025

Beijing, China



Subway Station
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Peking University
Exit C

For
Excursion

2DCOS XIII
Symposium
at Room A204
of Chemistry
Building A

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NO. 9 Building

Guesthouse
NO. 1 Building

Buffets on Aug.
17，18, and 19

North

Committes

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Prof. Isao Noda, University of Delaware, USA

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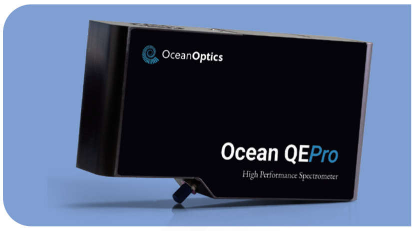

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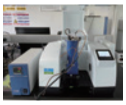		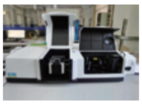	
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		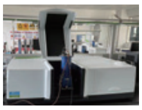	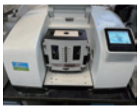
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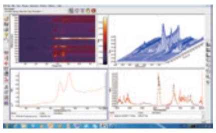

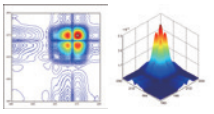

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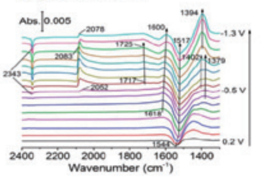

J. Am. Chem. Soc., 2017, 139(44): 15664–15667
DOI: 10.1021/jacs.7b10462

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The Program of the 2DCOS XIII Symposium

Registration

From 14:00-22:00， August 16, 2025

From 8:00-18:00, August 17, 2025

On-line Sessions for the 2DCOS XIII Symposium

Session 1 From 8:00AM to 13:30 PM (Beijing Time) on August 17, 2025

Zoom meeting - 2DCOS-13_SESSION 1

https://kangwon-ac-kr.zoom.us/j/82223891798

Session 2 From 14:00PM to 19:00 PM (Beijing Time) on August 17, 2025

Zoom meeting - 2DCOS-13_SESSION2

https://kangwon-ac-kr.zoom.us/j/82037510981

Session 3: From 8:00AM to 13:30 PM (Beijing Time) on August 18, 2025

Zoom meeting - 2DCOS-13_SESSION3

https://kangwon-ac-kr.zoom.us/j/83787428435

Session 4 From 8:00AM to 11:30 AM (Beijing Time) on August 19, 2025

Zoom meeting - 2DCOS-13_SESSION4

https://kangwon-ac-kr.zoom.us/j/82013265906

August 17, 2025

	Time		Mode	Type	Chair
	8:00-8:30	Open Ceremony			Hui-Zhou Liu
1	8:30-9:00	Isao Noda	On-line	Plenary Lecture	Yang Gao
2	9:00-9:30	Young Mee Jung	In-person	Plenary Lecture	Yu-Qing Wu
3	9:30-9:50	Zhi-Wu Yu	In-person	Invited Talk	
	9:50-10:00	Break			
4	10:00-10:20	Thomas G. Mayerhöfer	In-person	Invited Talk	Feng Gai
5	10:20-10:40	Hong Cheng	In-person	Invited Talk	
6	10:40-11:00	Bin Xia	In-person	Invited Talk	
	11:00-11:10	Break			
7	11:10-11:30	Thomas P. Burghardt	On-line	Invited Talk	Yang Gao (Lunch Time)
8	11:30-11:50	Wei Zhao	On-line	Invited Talk	
9	11:50-12:10	Andjelka B. Kovačević	On-line	Invited Talk	
10	12:10-12:30	Aleksandra Wesełucha-Birczyńska	On-line	Invited Talk	
11	12:30-12:50	Anna Kołodziej	On-line	Invited Talk	
12	12:50-13:10	In-Sang Yang	On-line	Invited Talk	
13	14:00-14:20	Gang Ma	In-person	Invited Talk	Zhi-Wu Yu
14	14:20-14:40	Yeonju Park	In-person	Invited Talk	
15	14:40-15:00	Huizhen Li	In-person	Invited Talk	
16	15:00-15:20	Yoonji Kim	In-person	Invited Talk	
	15:20-15:30	Break			
17	15:30-15:50	Ran Guo	In-person	Invited Talk	Thomas G. Mayerhöfer
18	15:50-16:10	Dongliang Tao	In-person	Invited Talk	
19	16:10-16:30	Jiwoo Cho	In-person	Invited Talk	
20	16:30-16:50	GuiMei Dong	On-line	Invited Talk	Yang Gao
21	16:50-17:10	Ying Liu	On-line	Invited Talk	
22	17:10-17:30	Lijuan Huang	On-line	Invited Talk	
23	17:30-17:50	Hai-long Feng	On-line	Invited Talk	
24	17:50-18:10	Carmen-Mihaela Popescu	On-line	Invited Talk	
25	18:10-18:30	Ljupcho Pejov	On-line	Invited Talk	
	18:30-20:30	Buffet			
	21:00-23:00	On-line Discussion: Zoom - 2DCOS-13(Aug. 17, 2025) – https://kangwon-ac-kr.zoom.us/j/85369569474			

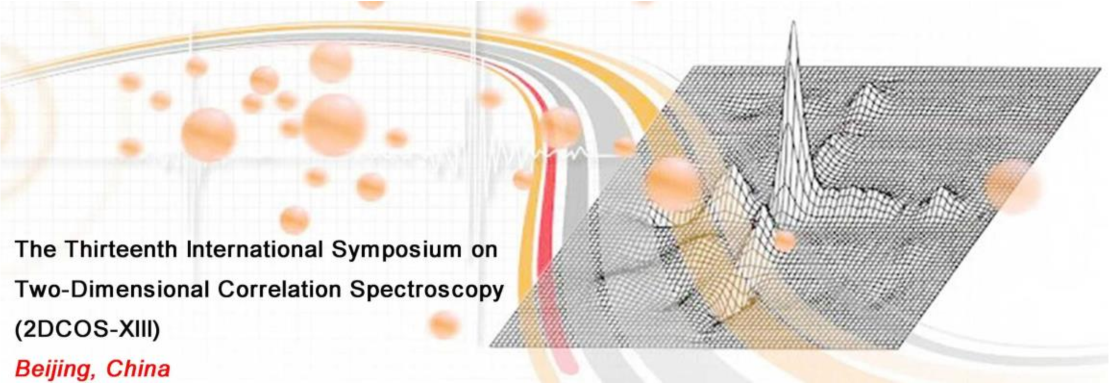
August 18, 2025

	Time		Mode	Type	Chair
26	8:00-8:30	Yukihiro Ozaki	In-person	Plenary Lecture	Young Mee Jung
27	8:30-9:00	Feng Gai	In-person	Plenary Lecture	
28	9:00-9:20	Hoeil Chung	In-person	Invited Talk	
	9:20-9:30	Break			
29	9:30-9:50	Edyta Proniewicz	In-person	Invited Talk	Dennis Hore
30	9:50-10:10	Yu-Qing Wu	In-person	Invited Talk	
31	10:10-10:30	Hong Yan Dai	In-person	Invited Talk	
32	10:30-10:50	Guanlin Lu	In-person	Invited Talk	
	10:50-11:00	Break			
33	11:00-11:20	Bogumiła Kupcewicz	On-line	Invited Talk	Yang Gao (Lunch Time)
34	11:20-11:40	Qiaolin Zhang	On-line	Invited Talk	
35	11:40-12:00	Zofia Chajdaś	On-line	Invited Talk	
36	12:00-12:20	Jia Long	On-line	Invited Talk	
37	12:20-12:40	Xi Li	On-line	Invited Talk	
38	12:40-13:00	Alberto Mezzetti	On-line	Invited Talk	
	14:00-18:00	Excursion			
	18:30-20:30	Buffet			
	21:00-23:00	On-line Discussion: Zoom meeting - 2DCOS-13(Aug. 18, 2025) https://kangwon-ac-kr.zoom.us/j/83981375750			

August 19, 2025

	Time		Mode	Type	Host
39	8:00-8:30	Dennis Hore	In-person	Plenary Lecture	Hoeil Chung
40	8:30-8:50	Yoshiteru Matsumoto	In-person	Invited Talk	
41	8:50-9:10	Xin Zhao	In-person	Invited Talk	
42	9:10-9:30	Linchen Xie	In-person	Invited Talk	
	9:30-9:40	Tea Break			
43	9:40-10:00	Juan Feng	In-person	Invited Talk	Yoshiteru Matsumoto
44	10:00-10:20	Xin Zhang	In-person	Invited Talk	
45	10:20-10:40	Kunjun Lu	In-person	Invited Talk	
46	10:40-11:00	Jianguo Chang	In-person	Invited Talk	
	11:00-11:20	Close Ceremony			Young Mee Jung
	11:20-	Lunch (buffet)			

abstracts of lectures



according to the number of presentation

Oral (L1)

RECENT PROGRESS IN TWO-DIMENSIONAL CORRELATION SPECTROSCOPY (2D-COS)

Isao Noda

Department of Materials Sciences and Engineering, University of Delaware, Newark, DE 19716, U.S.A.

The field 2D-COS has experienced a steady growth encompassing the utilization of vast arrays of spectroscopic probes, diverse perturbation methods to induce spectral intensity variations, and broad application areas, leading to a substantial number of scientific publications. An overview on the significant progress in the field especially in the last few years is reported. The state of this field seems to be healthy and vigorous with plenty of new developments. While the traditional 2D-COS has already proved itself to be a powerful and versatile technique, many other new modifications and improvements have also being reported. To further enhance the effectiveness and capability of 2D-COS and related techniques, several useful ancillary tools have recently been introduced. Some noteworthy techniques among them are highlighted.

Correlation filter is a technique to streamline the interpretation of often congested 2D correlation spectra comprising too many cross peaks by selectively attenuating interfering signals. The technique is more reliable and robust compared to the previously suggested method, like null space projection, which has the potential risk of over subtracting the interfering signals. 2D-COS carried out on the correlation filtered dataset can bring out more subtle details of the dynamics of minor constituents often obscured by the overwhelming presence of dominant signals. The utility of correlation filtering operation will be demonstrated on the analysis of rather challenging real world spectral dataset comprising elusive signals arising from a number of constituents with highly overlapped spectral features.

Identification of the characteristic bands, which exhibit the most distinct features (i.e., least correlated with each other) is often an important step in 2D-COS analysis, including the establishment of a proper set of correlation filters. Such bands have usually been selected by a subjective method, like simple visual inspection of correlation cross peaks. More systematic and reproducible hierarchical procedure is now developed based on the sequential multiplication of the horizontal slices of 2D spectra. Such an unsupervised automatic method may be potentially integrated into a model-free 2D-COS analysis compatible with the promising AI-based interpretation.

Oral (L2)

TWO-DIMENSIONAL CORRELATION SPECTROSCOPY IN SERS STUDIES

Shuang Guo[1,2], Yeonju Park[1], Lei Chen[3], Young Mee Jung[1,*]

[1]Department of Chemistry, Institute for Molecular Science and Fusion Technology, and
Kangwon Radiation Convergence Research Support Center, Kangwon National University,
Chuncheon 24341, Korea
(*ymjung@kangwon.ac.kr*)

[2]Key Laboratory of Preparation and Applications of Environmental Friendly Materials,
College of Chemistry, Jilin Normal University, Changchun 130103, China

[3]School of Materials Science and Engineering, Jilin Jianzhu University, Changchun. China

Two-dimensional correlation spectroscopy (2D-COS) is a powerful technique for analyzing spectral data influenced by external perturbations, offering deeper insights than conventional one-dimensional methods. It can uncover subtle molecular changes that are often undetectable in standard spectral analysis. Surface-enhanced Raman scattering (SERS), known for its exceptional sensitivity, selectivity, efficiency, and rapid, nondestructive detection, is a leading method in analytical spectroscopy. For detailed investigations of molecular interactions, surface phenomena, and enhancement mechanisms, we combined 2D-COS with SERS. This presentation will showcase the diverse applications of 2D-COS in SERS, emphasizing its strong analytical capabilities.

References

1. Qi Chu, Wei Wang, Shuang Guo, Eungyeong Park, Sila Jin, Yeonju Park, Lei Chen, Yucun Liu, Young Mee Jung “Interface Design of 3D Flower-like Ag@ZnSe Composites: SERS and Photocatalytic Performance” *ACS Appl. Mater. Interfaces* **2023**, 15, 11304-11313.
2. Shuang Guo, Yeonju Park, Eungyeong Park, Sila Jin, Lei Chen, Young Mee Jung “Molecular-Orbital Delocalization Enhances Charge Transfer in π-Conjugated Organic Semiconductors” *Angew. Chem. Int. Ed.* **2023,** e202306709
3. Yuenan Pan, Qi Chu, Shuang Guo, Sila Jin, Eungyeong Park, Yeonju Park, Yantao Sun, Lei Chen, Young Mee Jung, “Synergistic Contribution to the Enhanced Charge Transfer of the Silver/4-Mercaptobenzoic Acid/Polyaniline (Ag/MBA/PAN) System: Thickness-Dependent of PAN” *Appl. Surf. Sci.* **2022,** *586,* 152863.

Oral (L3)

Search for Liquid Clusters, Case Studies on Electrolytes

Jing Ma, Yaqian Wang, and Zhiwu Yu*

MOE Key Laboratory of Bioorganic Phosphorous Chemistry and Chemical Biology,
Department of Chemistry, Tsinghua University, Beijing 100084, P. R. China

The majority of liquids are inhomogeneous. It is believed that there exist various interaction complexes, or associates and clusters, in liquid mixtures/solutions. Identification of them, however, is challenging because of the dynamic nature of liquids. We have been working in this area in the last two decades. A method called excess spectroscopy was proposed. Also employed in our work is the well-developed two-dimensional spectroscopy (2D-COS). Both approaches have the merit to enhance apparent resolution of the collected molecular spectra. In this presentation, we will show our recent work on the cluster investigation of sodium and lithium electrolytes consisting of inorganic salts and neutral solvents. Following is an example of the 2D-COS results of the binary system consisting of sodium trifluoromethanesulfonate (NaOTf) and the neutral solvent 1,2-dimethoxyethane (DME).

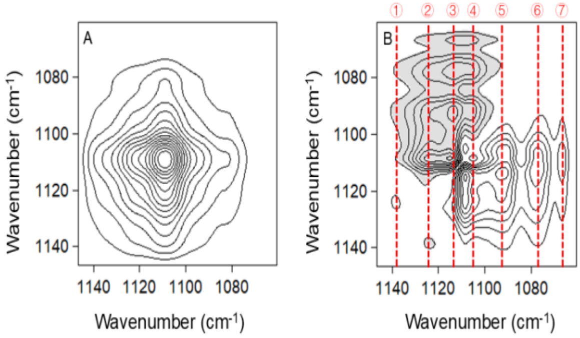


Figure 1. The synchronous (A) and asynchronous (B) 2D-COS spectra contour maps in the region of v(C-O-C). White and gray backgrounds represent positive and negative correlation intensities, respectively.

Combining 2D-COS and excess spectroscopy and assisted with quantum chemical calculations, promising clusters are identified. The work may shed lights on the in-depth understanding of the working mechanism of battery electrolytes.

Oral (L4)

QUANTIFYING SPECTRAL NONLINEARITY USING COMPLEX-VALUED CLASSICAL LEAST SQUARES REGRESSION AND 2D-CORRELATION ANALYSIS

Thomas G. Mayerhöfer,[1,2] *Isao Noda*,[3] *Juergen Popp*[1,2]

[1] *Leibniz Institute of Photonic Technology (Leibniz-IPHT), Jena, Germany*
[2] *Institute of Physical Chemistry and Abbe Center of Photonics, Friedrich Schiller University, Jena, Germany*
[3] *University of Delaware, Newark, USA*

The Bouguer-Beer-Lambert law is typically regarded as a fundamental principle, describing a linear relationship between absorbance, molar concentration, and the optical path length through a sample. However, its three namesakes developed their work before the advent of Maxwell's equations—at a time when light was not yet recognized as electromagnetic radiation capable of polarizing matter. As a result of this polarization, the relationship between absorbance and concentration is only approximately linear.[1]

We previously demonstrated this deviation qualitatively using 2D correlation analysis.[2] By combining 2D correlation with "smart error sums," the effect can now also be quantified.[3] The results are compared with those obtained from complex-valued Classical Least Squares (CV-CLS) regression. To this end, we used modeled spectra of a hypothetical thermodynamically ideal mixture obeying the Lorentz-Lorenz relation, yielding systematic errors that resemble those observed in real mixtures.

Interestingly, in CV-CLS, such systematic errors manifest in the volume fractions as complex numbers. The imaginary component can be used to reduce the overall error—by up to 25% or more—when CV-CLS is used instead of conventional CLS for experimental spectra. Complex-valued tools such as 2D correlation and chemometric regression methods promise to enhance the spectroscopic toolbox by introducing phase-sensitive, complex-valued methodologies for the next generation of spectral analysis.

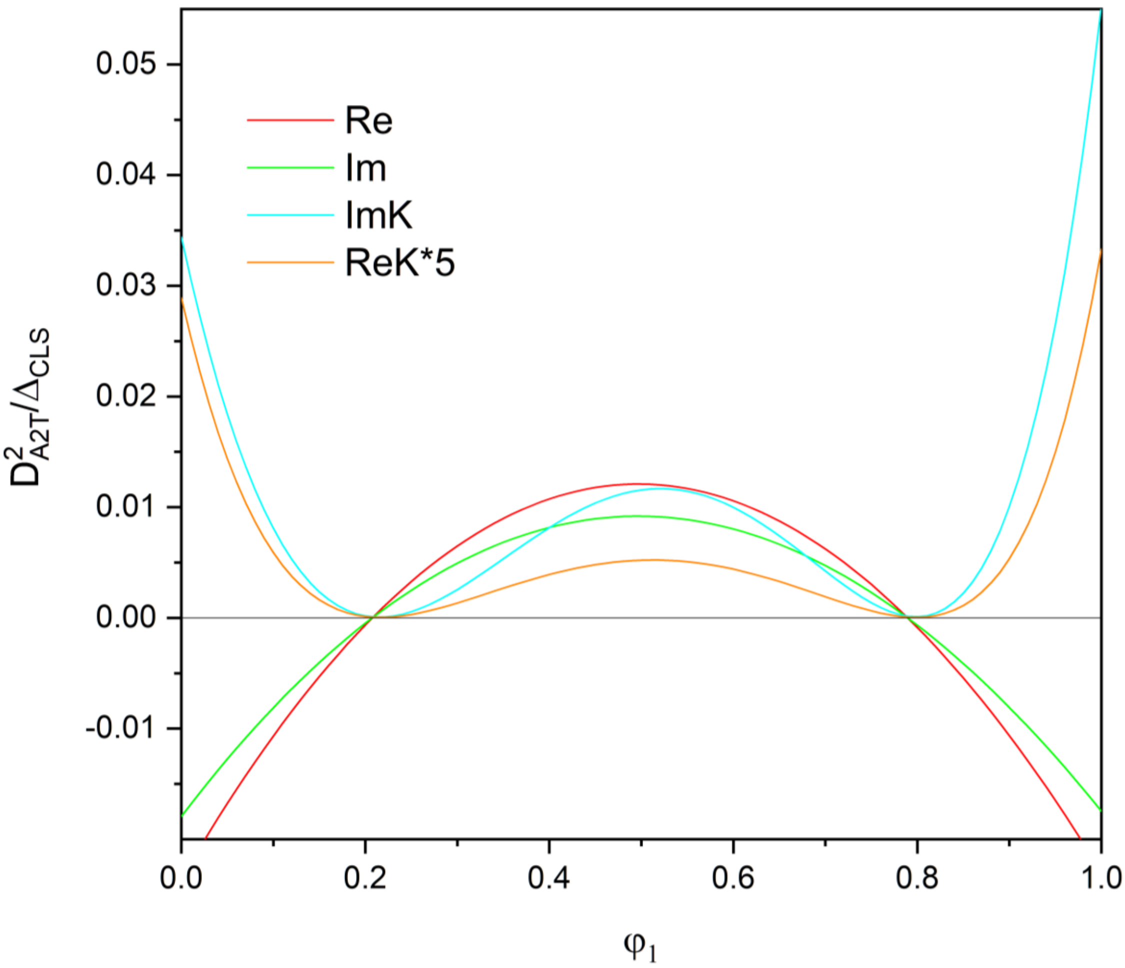


Fig. 1: Comparison between the errors of CV-CLS and those determined by employing the 2T2D-smart error sum to a series of spectra of a hypothetical thermodynamically ideal mixture obeying the Lorentz-Lorenz relation.

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Financial support from the EU, the ”Thüringer Ministerium für Wirtschaft, Wissenschaft und Digitale Gesellschaft”, the ”Thüringer Aufbaubank”, the Federal Ministry of Education and Research, Germany (BMBF), the German Science Foundation, the “Fonds der Chemischen Industrie” and the Carl-Zeiss Foundation is gratefully acknowledged.

Oral (L5)

APPLICATION OF HYPERSPECTRAL IMAGING IN QUALITY DETECTION OF PEAR FRUITS

Hong Cheng,[1] Jian-Ping Zhang[2]

[1] Institute of Biotechnology and Food Science, Hebei Academy of Agriculture and Forestry Sciences, Shijiazhuang 050051, Hebei, China
[2] Key Laboratory of Advanced Light Conversion Materials and Biophotonics, School of Chemistry and Life Resources, Renmin University of China, Beijing 100872, China

Fruit and vegetable quality is a key determinant of market value and consumer satisfaction, thereby playing a crucial role in global agriculture and the food industry. Consequently, developing effective strategies for quality assessment is essential for improving product quality. Hyperspectral imaging (HSI) has emerged as a powerful, non-destructive, accurate, and rapid tool for evaluating quality attributes in agricultural products. HSI has been widely used to predict internal quality parameters and detect external disorders in fruits and vegetables[1]. In this study, we first applied visible and near-infrared HSI combined with machine learning algorithms to accurately predict α-farnesene and conjugated trienol contents, key indicators of superficial scald in ‘Yali’ pear[2]. Subsequently, we used HSI to predict chlorophyll fluorescence parameters, which serve as reliable indicators for assessing senescence in green ‘Yali’ pear, yielding excellent predictive performance[3]. Furthermore, by increasing the sample size, we significantly improved the accuracy of HSI models for non-destructively estimating seven quality attributes (firmness, SSC, pH, L^*, a^*, b^*, and I_{AD}) across six pear cultivars[4]. Overall, this study demonstrates the broad potential of HSI for evaluating both internal and external quality attributes in pears.

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Oral (L6)

DNA Binding Mechanism of the Virulence Regulator SarA of Staphylococcus aureus

Bin Xia

Beijing Nuclear Magnetic Resonance Center, Peking University, Beijing, 100871, China

Staphylococcus aureus infections have long been a significant challenge to public health, particularly due to the emergence of multiple drug-resistant strains. SarA is a critical global regulator in *S. aureus* which binds to AT-rich sequences in the promoter regions of various genes, but the DNA-binding mechanism of SarA remains unclear.

We have determined the solution structures of a monomeric DNA binding domain of SarA (SarA$^{\Delta N19}$) and its complex with an AT-rich double-stranded DNA. The winged helix domain of SarA$^{\Delta N19}$ binds to DNA in a classic way, with the α4 helix binding to the major groove of DNA, while the L5 loop binding to the minor groove, covering 10 AT base pairs. Residues L53, P65, and V68 of the α4 helix have hydrophobic interactions with thymine bases and sugar rings. The side chains of Arg90 and Arg84 from the wing are inserted into the minor groove, forming hydrogen bonds with A/T bases. Multiple positively charged or hydrophilic residues, including Lys54, Lys63, Lys69, Lys72, Lys82, and Gln64, interact with the phosphate groups on the DNA backbones.

This complex structure provides an in-depth understanding of the molecular mechanism for SarA to bind DNA, and a structure basis forthe anti-bacterial drug design targeting SarA.

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Oral (L7)

Two-dimensional correlation genetics reveals mechanisms for inheritable heart diseases in cardiac ventriculum

Thomas P. Burghardt
Department of Biochemistry and Molecular Biology, 200 First St. SW, Mayo Clinic Rochester, Rochester, MN, 55905, USA

1. Background

Muscle proteins assembled in the sarcomere produce force and displacement by their coordinated action. In human ventriculum, cardiac myosin (βmys) and actin form interdigitated thick- and thin-filaments with βmys ATPase motor domains extending outward from the thick-filament backbone in regular helical arrays to contact thin-filament actin. βmys repetitively converts ATP free energy into work by translating the thin-filament against resisting force. A subset of myosins form a complex with a regulator called myosin binding protein C (MYBPC3). MYBPC3 regulates muscle activity through inter-protein contacts among domain sub-structures in the actin/βmys/MYBPC3 complex. The focus here is on βmys/MYBPC3 inter-protein contacts.

2. Method

Single residue variants (SRVs) alter the native protein sequence in βmys or MYBPC3 sometimes causing inheritable heart disease. Muscle protein genetics encode instructions for the contraction mechanism informing protein construction, systemic functional integration, and inheritable disease functional impairment. A neural-network contraction model characterizes SRV impact on human health. It rationalizes phenotype and pathogenicity assignment given SRV characteristics and, in this sense, decodes the βmys/MYBPC3 complex genetics to implicitly capture ventricular muscle functionality [1, 2]. When an SRV modified domain locates to an inter-protein contact in the βmys/MYBPC3 complex it affects the complex coordination. Domains involved, one in βmys and the other in MYBPC3, form coordinated-domains (co-domains). Co-domain formation implies potential for their SRV modification probabilities to respond jointly to a common perturbation revealing location. Worldwide human genetic divergence attributed to human migration from a single origin in East Africa is based on the serial founder effect addressing migration [3], colonization, and exchange between geographically near populations [4]. The serial founder effect explains an observed linear divergence decrease with human migration distance over the earth's surface making migration distance a proxy for genetic divergence variation. Linearly decreasing genetic variation consistent with the serial founder effect is likewise detected in the Single Nucleotide Polymorphism (SNP) database (a super-set of the SRV database) independently confirming the worldwide genetic variation trend [5]. Genetic diversity is the systemic perturbation coupling co-domains mapped with two-dimensional correlation genetics (2D-CG).

3. Results

2D-CG co-domain mapping gives structural insight into co-domain function expressed in natural language format. It exploits the implicit machine-learned intelligence from the neural network model by providing human accessible insight based on the 2D-CG map. The latter combined with other pertinent data from the literature forms a neural-symbolic hybrid model integrating genetic and protein-interaction data into a nascent digital twin. The process, outlined in **Figure 1**, is a template for combining different datasets, in this case genetic and structural, into an evolving model for disease mechanism [2].

Figure 1 shows the neural-symbolic hybrid model for βmys/MYBPC3 complex in cardiac ventriculum. Bootstrap section uses a simplified neural network model for the βmys/MYBPC3 complex requiring only the SNP (genetic) database to provide the training dataset. A Human Data Miner agent integrates the Bootstrap 2D-CG co-domain contacts with structural data from the literature to develop the advanced neural network model and training dataset that includes filament structure. Filament structure defines the force producing actomyosin interaction making it a key determinant for disease mechanism and begins the virtuous-cycle.

The virtuous-cycle iteration supplies revised co-domains identified in the 2D-CG Optimized Contacts map. **Figure 1** has two co-domain pairs identified with large yellow arrows in the cartoon structure representing myosin dimers in adjacent human cardiac myosin thick-filaments interacting with MYBPC3. The latter is depicted schematically as a gray polypeptide chain connecting spherical domains c0 through cx. Thick filament structure was surmised by interpreting a cryo-EM reconstruction in the presence of mavacamten [6]. Myosin dimers form blocked (red) and free (blue) heads within the interacting-heads motif (IHM). Blocked heads have their actin binding site blocked by a specific interaction with the free head partner. Interacting heads in the IHM are folded onto the helical myosin filaments in a relaxed muscle forming a super-relaxed state (SRX). The SRX state inhibits free head myosin contact with actin preventing force development. In contrast, a disordered-relaxed state (DRX, not indicated in **Figure 1**) exhibits force development by allowing actin to contact myosin head (specifically motor) domains. Head domains shown also include bound essential (green) and regulatory (yellow) light chains.

SRX structure (shown) is the starting point for representing scenarios for co-domain interactions consistent with 2D-CG for SRV's associated with dilated cardiomyopathy (DCM) [2]. DCM disease causes ventricular wall weakness and declining pump efficiency probably because few myosin heads can make actin contact when locked in the SRX state. DCM induced co-domains from one MYBPC3 polymer with two myosin head domains across different filaments imply an enhanced myosin head sequestering from actin contact consistent with DCM phenotype (i.e., a "super"-SRX state) possibly akin to hyper-relaxed motor domains [7]. **Figure 1** illustrates this scenario with DCM SRVs in myosin or MYBPC3 linking loop 3 (L3) in the actin binding region on the free head from crown level CrT in the myosin thick-filament (top) with MYBPC3 C-terminus cx domain, and, actin binding C-Loop (CL) on an adjacent myosin filament (right) at the blocked head in CrD with MYBPC3 phospho-threonine 8 (s8 or Thr607) between c4 and c5 domains. Other scenarios are consistent with existing co-domain maps. Work in progress enhances co-domain mapping resolution by involving larger and broader human SRV datasets and thin-filament actin.

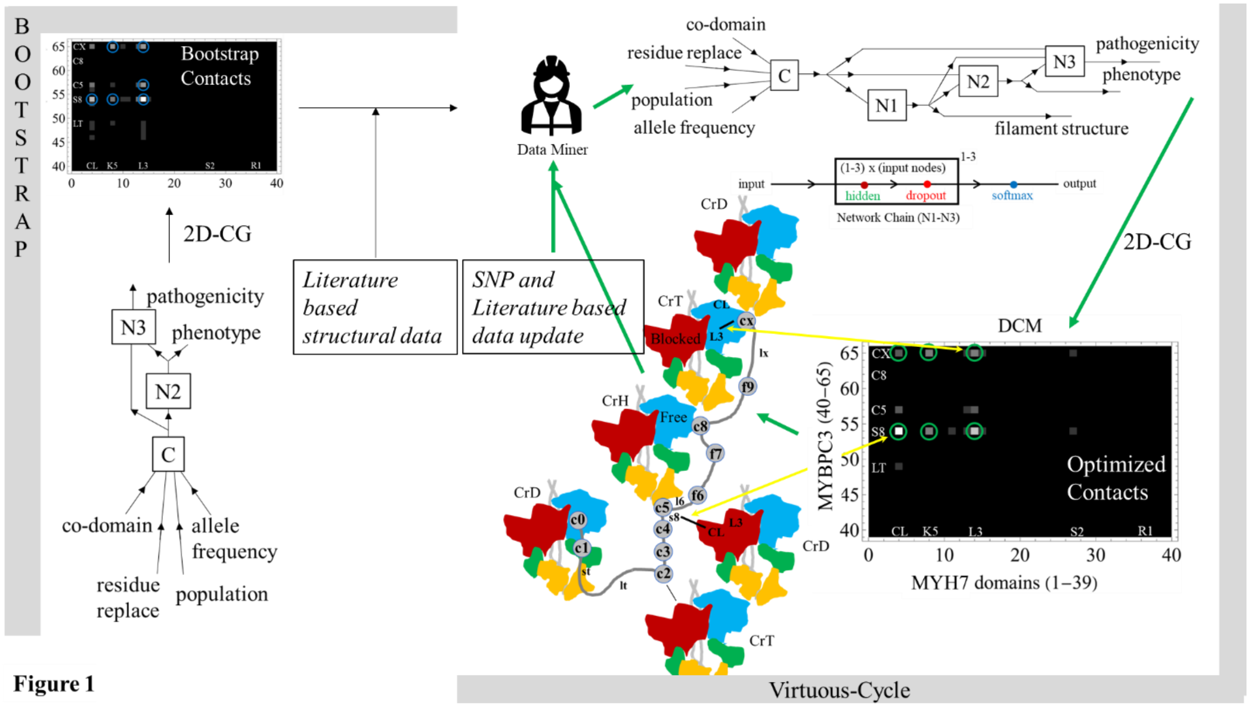

Figure 1

Familial hypertrophic cardiomyopathy (FHC) disease causes cardiac wall thickening to inhibit pumping efficiency probably related to disrupted head sequestering. In this case the DRX state prevails (i.e., a "super"-DRX state) where too many heads bind actin. It abnormally thickens cardiac ventricular walls leading to declining pump efficiency. An observed distinction between co-domains favored in FHC and DCM phenotypes show that they distinguish inheritable diseases thus intimating disease mechanisms [2].

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Oral (L8)

Simulation of Doubly Vibrationally Enhanced (DOVE) Four Wave Mixing Spectroscopy of Water Monomers

Wei Zhao

School of Physical Sciences, University of Arkansas at Little Rock, Little Rock, AR 72204, United States

Water is an interesting but challenging model system for the development of doubly vibrationally enhanced (DOVE) four wave mixing spectroscopy, an optical analogue to 2D NMR. DOVE four wave mixing spectroscopy involves two infrared transitions and a Raman transition.[1] The magnitude of the DOVE second hyperpolarizability can be theoretically estimated if the values of the dipolar moments of the two infrared transitions and the γ of the Raman transition are known. We have demonstrated that the second hyperpolarizability γ value of a selected vibrational mode of a molecule can be determined by using the computational Raman activity against an internal standard with a known Raman γ value.[2-4] This approach provides a facile way for prediction of the magnitude of DOVE signals.[5] By using the Hartree-Fock (HF) method and the DFT method, here we have estimated the magnitude of the DOVE second hyperpolarizability of water monomers and identify the strong water DOVE signatures at the cross peaks (ν_2, $\nu_2 + \nu_3$) and (ν_1, $\nu_1 + \nu_3$), useful for label-free molecular determination in a complex system.

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Oral (L9)

AI-ENHANCED QUASAR HARMONIC EXPLORER: A FRAMEWORK FOR SIGNAL DISENTANGLEMENT IN NOISY ASTROPHYSICAL TIME SERIES

Andjelka B. Kovačević

University of Belgrade – Faculty of Mathematics, Department of Astronomy
Studentski trg 16, 11 000 Belgrade, Serbia

We present recent work on an AI-integrated framework that enhances the capabilities of the Quasar Harmonic Explorer (QhX), a signal analysis tool designed to identify multiperiodic and non-sinusoidal features in red noise-dominated time series [1]. Originally developed for analyzing quasar variability in active galactic nuclei (AGN), QhX now incorporates neural architectures to extract robust temporal representations from irregular and noisy light curves. Drawing inspiration from the principles of two-dimensional correlation spectroscopy (2DCOS, [2]), we transform time-domain astrophysical data into time–frequency and cross-correlation maps that serve as input to deep learning models, enabling analogies with synchronous and asynchronous 2D correlation spectra. We demonstrate relevance to 2DCOS-style problems by highlighting parallels between multi-band quasar light curves and multidimensional spectroscopic data, showing how similar AI-driven disentanglement techniques can be adapted to analyze complex vibrational spectra and correlated spectral responses in other domains. This work exemplifies the convergence of astronomy, spectroscopy, and machine learning, showcasing how AI can bridge complex signal environments across disciplines.

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Oral (L10)

2D-COS EXTENDS AND DEEPENS THE INFORMATION ENCODED BY INDIVIDUAL ANALYTICAL METHODS

Aleksandra Wesełucha-Birczyńska[1], Maria Pajda[2], Elżbieta Długoń[3], Krzysztof Morajka[1], Marek Michalec[1], Marta Błażewicz[3]

[1]*Faculty of Chemistry, Jagiellonian University, Kraków, Poland*

[2]*Technolutions, Łowicz, Poland*

[3]*AGH – University of Science and Technology, Faculty of Materials Science and Ceramics, Kraków, Poland*

Membranes made of carbon nanofibers (ESCNFs) are interesting new generation materials. Manufacturing processes that typically use electrospinning have a significant impact on their structure and properties[1-3]. Therefore, they are promising materials with tailored properties for a medical, industrial and other applications. Even though work on these materials has been going on for some time, their mechanical properties have not been fully understood, and from the point of view of medical applications, there is still no coherent theory that would explain their effect on living organisms.

The membranes made of carbon nanofibers (ESCNF): an unmodified membranes as a reference samples, then subjected to chemical and thermal treatment, were analyzed. These processes lead to a significant reconstruction of the molecular structure. The Raman microspectroscopy technique was used to obtain spectra of the studied membranes excited with laser lines of wavelengths of 442 nm, 514.5 nm and 785 nm. The 2D correlation analysis was performed using the Raman spectra obtained with different laser line energies as the perturbation input to generate correlation maps[4]. The X-ray diffraction data of these membranes were collected on the Philips diffractometer type X'Pert Pro in the Bragg-Brentano geometry, using CuKα radiation ($\lambda = 0.154184$ nm). Diffraction patterns indicate amorphization of materials and/or different crystalline phase formation. The nanoindentation method clearly differentiates the tested samples, e.g. the instrumented hardness or plasticity[5]. 2D-COS correlation of the Raman spectra leads to the unraveling of the hidden phases and the determination of the mechanical properties characterizing the tested materials.

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Oral (L11)

TWO-DIMENSIONAL CORRELATION AS A TOOL FOR EARLY ASSESSMENT OF THE MATERIAL'S BIOACTIVITY

A. Kołodziej[1], M. Świętek[2], Ł. Skalniak[1], M. Gubernat[3], A. Wesełucha-Birczyńska[1]

[1] Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387 Kraków, Poland
[2] Institute of Macromolecular Chemistry, Czech Academy of Sciences, Heyrovského nám. 2, 162 06 Prague 6, Czech Republic
[3] Faculty of Materials Science and Ceramics, AGH University of Krakow, B-8, Adama Mickiewicza 30/0.24, 30-059 Kraków, Polska

A generally accepted method for bioactivity assessment of materials is cell proliferation test. However, it provides information mainly about changes in cell populations, not cellular interactions with material surface. Previously, studies regarding the polymer composites characteristics and bioactivity were performed. Membranes made of polycaprolactone and nanocarbon additives such as reduced graphene oxide, and graphene oxide underwent structural analysis and bioactivity tests.[1,2] The use of nanocarbon structures in medicine is a hot topic, given previously contradictory scientific reports that consider them, on the on hand, bioactive and osteoinductive, while on the other hand, highly toxic to living organisms. The studies presented are extremely important for expanding knowledge about the biological properties of nanocarbon structures. Raman spectroscopy facilitated the recognition of crystallinity and ordering of polymer chains, providing molecular-level insights into the interactions between the nanoadditive and the polymer. The *in vitro* U-2 OS cell assay was combined with simultaneous Raman measurements of single cells on the material surface at the consecutive days of the cell proliferation test and analysis via two-dimensional correlation analysis. Differences in cellular responses to the two types of materials were categorized as early as the first week of the proliferation test by 2D-COS analysis, while the fluorescence microscopy technique was able to distinguish the differences only after two weeks. Therefore, the cell growth on material combined with Raman spectroscopy measurements and 2D-COS analysis is a proposal of an innovative, early assessment tool of the material's bioactivity.

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Oral (L12)

2D correlation spectroscopy analyses of the spin-rotational excitations in hexagonal $YMnO_3$

Young-Jin Lee[1], Yeonju Park[2], Young Mee Jung[2], Je-Geun Park[3], In-Sang Yang[1,*],

[1] *Department of Physics, Ewha Womans University, Seoul 03760, Korea*

[2] *Department of Chemistry, Institution for Molecular Science and Fusion Technology, Kangwon Radiation Convergence Research Support Center, Kangwon National University, Chuncheon, 24341, Korea*

[3] *Department of Physics and Astronomy, Seoul National University, Seoul 08826, Korea*

Two-dimensional correlation spectroscopy (2D-COS) analyses are performed on the temperature-dependent Raman peaks of hexagonal $YMnO_3$ single crystals. Under the resonance with the on-site Mn *d*-*d* transitions, the spin excitation peaks are observed at 550 and 780 cm^{-1}, and they are believed to be due to spin rotations by 120° and 180° of the Mn-ion spins in a trimer in the antiferromagnetic ordered state.[1] 2D-COS analyses on the broad peak ~ 780 cm^{-1} show that there exist several components in the spin-rotational excitation peaks. This results suggest the variations in spin symmetries in the AF ordered ground state of $YMnO_3$.

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The measurements were supported by Korea Basic Science Institute grant funded by the Ministry of Education (2020R 1A 6C 101B194), and ISY was financially supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education (2021R1A6A1A10039823).

Presenter : In-Sang Yang: yang@ewha.ac.kr

Young-Jin Lee : youngjin@ewha.ac.kr

Yeonju Park : yeonju4453@kangwon.ac.kr

Young Mee Jung : ymjung@kangwon.ac.kr

Je-Geun Park : jgpark10@snu.ac.kr

Oral (L13)

SELF-ASSEMBLY OF Aβ-DERIVED SHORT PEPTIDES INVESTIGATED BY FTIR SPECTROSCOPY AND NONLINEAR OPTICAL SPECTROSCOPY

Gang Ma*
Key Laboratory of Medicinal Chemistry and Molecular Diagnosis of Ministry of Education, Key Laboratory of Analytical Science and Technology of Hebei Province, State Key Laboratory of New Pharmaceutical Preparations and Excipients, College of Chemistry and Materials Science, Hebei University, Baoding 071002, China

Short peptides derived from Alzheimer's disease-related Aβ peptides can self-assemble into various nanostructures, showing great potential in numerous practical applications.[1-5] Understanding their self-assembly behaviors is therefore of critical importance. This talk will explore the self-assembly structures and nucleation and growth mechanisms, as well as the interactions between self-assembled structures and biological membranes, of several short peptide systems derived from Aβ. Specifically, the following topics will be covered: (1) using FTIR spectroscopy to explore the non-amyloid structural characteristics of FF nanotubes; (2) employing side-chain-based infrared probe technique to investigate the nucleation and growth mechanisms of the self-assembly of KLVFFAK-related and Boc-FF-related systems; (3) utilizing second harmonic generation (SHG) and sum frequency generation vibrational spectroscopy (SFG-VS), as well as SEM and AFM, to investigate the interactions between FF nanotubes and phospholipids. It is hoped that these studies will deepen our understanding of the important phenomenon of peptide self-assembly.

* Corresponding author (gangma@hbu.edu.cn)

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Oral (L14)

MOLECULAR-LEVEL INSIGHTS INTO STIMULI-RESPONSIVE AND BIODEGRADABLE POLYMERS USING 2D CORRELATION SPECTROSCOPY

Yeonju Park[a,b], Sujin Lee[b], Siwoo Kim[b], Isao Noda[c], Young Mee Jung[a,b,*]

[a]Kangwon Radiation Convergence Research Support Center, Kangwon National University,
Chuncheon 24341, Korea

[b]Department of Chemistry, Institute for Molecular Science and Fusion Technology, Kangwon
National University, Chuncheon 24341, Korea

[c] Department of Materials Science and Engineering, University of Delaware, Newark, DE
19716, USA

**Corresponding author's E-mail: ymjung@kangwon.ac.kr*

Understanding the molecular moieties of polymers through spectroscopic analysis is crucial. However, the inherent complexity of polymer spectra often makes direct interpretation challenging. Two-dimensional correlation spectroscopy (2D-COS) offers a powerful approach to unraveling such complexity by providing enhanced spectral resolution and molecular-level insights. In this study, we applied 2D-COS and principal component analysis (PCA) to investigate temperature- and composition-dependent IR spectra of poly(*N*-isopropylacrylamide) and its stimuli-responsive derivatives, as well as poly(hydroxybutyrate-*co*-hydroxyhexanoate) and its biodegradable derivatives. Details of the results will be discussed in this presentation.

Oral (L15)

IMPROVING AQUEOUS MG-AIR BATTERY DISCHARGE PERFORMANCE VIA *a*-AMINO ACIDS ELECTROLYTE ADDITIVES

Hui-Zhen Li [a, *], Jie-hao He [a], Juan Cao [a], Yan-xin Deng [a], Qiu-Hao Chen [a], Liang-Ming Gao [a], Jun-Jie Yang [c,d], Xing-Peng Guo [a, b], Bo-Kai Liao [a, b], *

a. *School of Chemistry and Chemical Engineering, Guangzhou University, Guangzhou, 510006, P.R. China*
b. *Joint Institute of Guangzhou University & Institute of Corrosion Science and Technology, Guangzhou University, Guangzhou, 510006, P.R. China*
c. *Institute of Advanced Wear & Corrosion Resistant and Functional Materials, Jinan University, Guangzhou, 510632, P.R. China*
d. *Shaoguan Research Institute of Jinan University, Shaoguan, 512027, P.R. China*

* Corresponding authors: lihz@gzhu.edu.cn; bokailiao@gzhu.edu.cn

ABSTRACT

Aqueous Mg-air batteries have applications in many areas such as energy storage, portable electronic device and automotive power system. However, their large-scale commercialization is hindered by poor discharge performance. In this study, histidine and alanine were introduced as eco-friendly electrolyte additives to enhance the electrochemical properties of Mg-air battery. Through comprehensive electrochemical measurements, H_2 evolution tests, morphological/compositional characterizations, and theoretical calculations, we systematically investigated the influence of the two *a*-amino acids on battery performance and their underlying reaction mechanisms. The results revealed that both additives effectively coordinate with Mg^{2+} and promote sustained Mg anode dissolution (Fig. 1). As a consequence, the discharge performance of aqueous Mg-air batteries was significantly enhanced. This work presents a feasible and eco-friendly strategy to advance Mg-air battery technology, paving the way for broader practical applications.

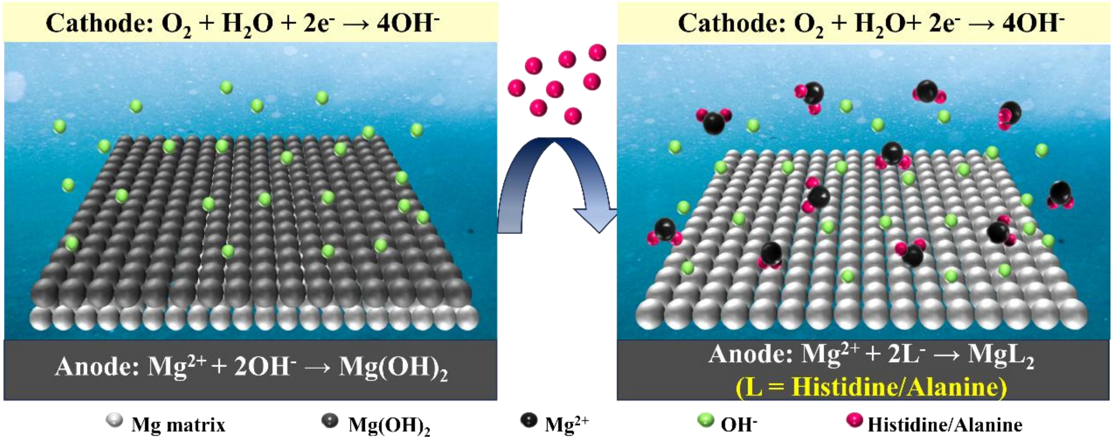


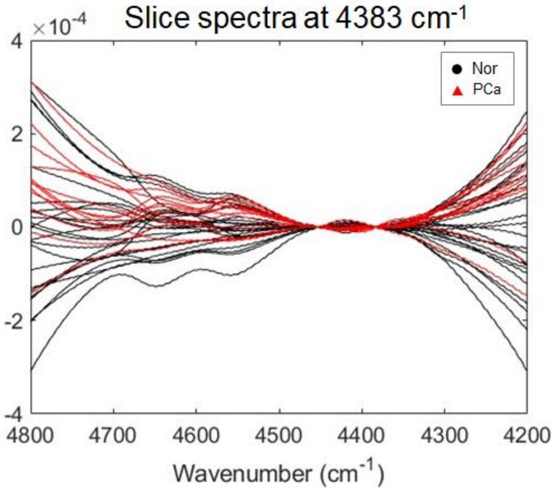
Fig. 1. Illustration of the reaction mechanism of amino acids with the Mg anode

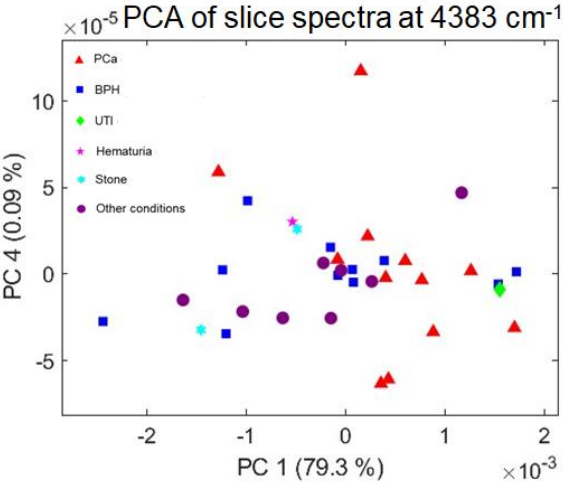
Oral (L16)

NEAR-INFRARED SPECTROSCOPIC INVESTIGATION OF DIVERSE UROLOGICAL DISEASES INCLDUING PROSTATE CANCER USING TWO-TRACE TWO-DIMENSIONAL ANALYSIS

Yoonji Kim and Hoeil Chung
Department of Chemistry, Hanyang University, Republic of Korea

Early detection of prostate cancer (PCa) is crucial for improving treatment outcomes, highlighting the need for rapid and non-invasive diagnostic methods. In this study, we employed near-infrared (NIR) spectroscopy combined with two-trace two-dimensional (2T2D) correlation analysis to investigate different urological diseases including PCa. For this purpose, the urine samples of 23 non-PCa and PCa patients were obtained and the corresponding transmission NIR spectra in the 4800–4200 cm^{-1} were acquire using a liquid cell. To potentially highlight metabolic differences among the samples better, the pH of each sample was separately adjusted to 2 for the spectral acquisition. It was a hope that cancer progression alters the composition metabolites in urine (body fluid), which in turn affects the surrounding environment of water-network and alter the spectral feature of corresponding water peak. When principal component analysis (PCA) was performed using the slice spectra at 4383 cm^{-1}, the scores of PCa against those of other diseases (benign prostatic hyperplasia (BPH), urinary tract infection (UTI), and hematuria) were somewhat separable, while the distinction needed to be improved further. For this, more effective chemometric tools to extract relevant information from the broad water peaks are required. Also, normal urine samples obtained from healthy subject without urological diseases should be employed as a control for deeper comparison.





Oral (L18)

SYNTHESIS AND CHARACTERIZATION OF A FLUORESCENT COMPOSITE BASED ON TERBIUM SALICYLATE COMPLEX AND HYDROXYAPATITE

Ziqi Xu[1], Haijun Zhu[1], Dongliang Tao[1]
Department of Chemistry & Materials Engineering, Fuyang normal university,
Fuyang, 236037, P.R.China

Persistent challenges of high production costs and low quantum yield hindered widespread application of terbium rare-earth complexes[1]. To address this, a low-cost composite fluorescent material was controllably synthesized using Tb^{3+} as the central ion coordinated with salicylic acid ligands on a hydroxyapatite (HAP) matrix functioning as both alkaline source and structural core. The HAP-promoted coordination between salicylic acid carboxyl groups and Tb^{3+} was confirmed by disappearance of the carboxyl C=O stretching peak at 1655 cm^{-1}. Complementary evidence included: (i) XRD detection of HAP characteristic peaks ($2\theta = 32.04°$, Fig. 1c), and (ii) EDS verification of terbium-containing species on HAP surfaces (Fig. 1d), collectively indicating a HAP-core/core-shell structure. Under optimal conditions (90°C/4 h/3 mmol DMF/2 g HAP), maximum emission intensity reached 1,155,000 CPS despite a limited quantum yield of 28.82%. Modified conditions (6 h/4 g HAP) reduced intensity to 710,398 CPS but increased quantum yield to 36.69%, while achieving 55.89% cost reduction versus pure Tb(SA)$_3$ complexes—significantly enhancing application prospects for rare-earth fluorescent materials.

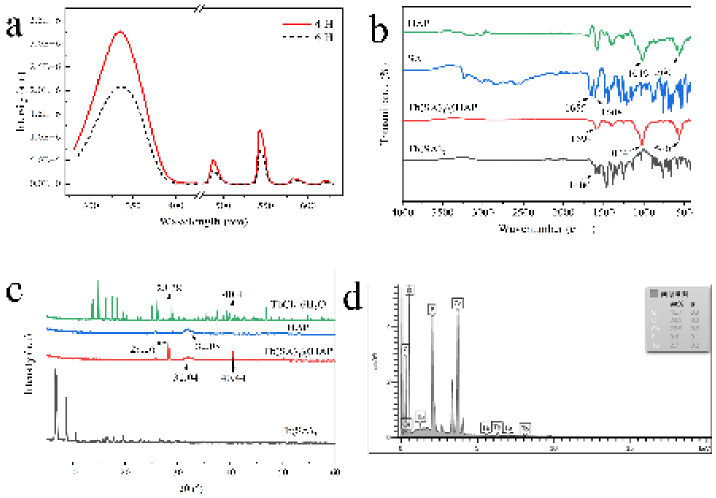


Fig 1. (a) Fluorescence spectrum of the Tb(SA)$_3$DMF@HAP; (b) FTIR spectrum; (c) XRD pattern. (d) EDS image of the Tb(SA)$_3$DMF composite.

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Oral (L19)

DISCRMINATION OF NATURAL AND LAB-GROWN DIAMONDS USING RAMAN SPECTROSCOPY COMBINED WITH TWO-TRACE TWO-DIMENSIONAL CORRELATION ANALYSIS

Jiwoo Cho[a], Yeseo Joo[b] and Hoeil Chung[a,*]

[a]*Department of Chemistry and Research Institute for Convergence of Basic Science,*
Hanyang University, Seoul 04763, Republic of Korea

[b]*Department of Materials Science & Engineering, The Graduate School of Engineering*
Hanyang University, Seoul 04763, Republic of Korea

The accurate discrimination of natural and lab-grown diamonds is critically required to assess their commercial values since natural diamonds are considerably more expensive in actual jewel markets. As a potential tool for the discrimination, Raman spectroscopy has been explored in this study since its measurement is simple and non-destructive and diamond has a strong and sharp Raman peak at 1332 cm^{-1}. As a preliminary study, Raman spectra of 15 natural and 15 lab-grown diamonds were collected and their spectral features were comparatively analyzed. For all the measured samples, the characteristic diamond peaks at 1332 cm^{-1} were noticed, while their intensities, widths, and positions were minutely dissimilar to each other. These spectral differences were obviously representative of varied lattice structures of natural and lab-grown diamonds. To sensitively highlight the minute spectral differences, two-trace two-dimensional (2T2D) correlation analysis was performed to the sample spectra and subsequent 2T2D slice spectra were examined. When principal component analysis (PCA) was performed using the slice spectra, the scores of natural and lab-grown diamonds were fairly separable, thereby demonstrating the feasibility of Raman spectroscopy-based discrimination. More diamond samples are under collection and analysis to provide more reliable assessment of the proposed Raman scheme. Also, infrared (IR) spectroscopy, an alternative method effective for the discrimination, will be employed and corresponding discrimination result will be mutually compared.

Oral (L20)

A REVIEW ON TWO-DIMENSIONAL CORRELATION SPECTROSCOPY APPLICATION IN MICROPLASTIC RESEARCH

Ren-Jie Yang, Gui-Mei Dong*, Jia Long, Ji-yuan He
College of Engineering and Technology, Tianjin Agricultural University, Tianjin, 300384
*guimeidong@gmail.com

Microplastics (MPs), as an emerging pollutant, have become a potential threat to the global ecological environment and human health due to their small particle size, wide distribution, easy interaction with other pollutants in the environment, and transmission through the food chain. Two-dimensional correlation spectroscopy (2D-COS) is an analysis method based on spectral response, which introduces external perturbations to obtain information on intermolecular interactions and dynamic changes, and exhibits unique advantages in microplastic research. The focus of this review is the application of 2D-COS technology in characterizing the chemical structure and functional groups of MPs, the aging and degradation mechanisms of MPs, the interactions between MPs and other pollutants, and the distribution and traceability of MPs in environmental media. Finally, the requirements and limitations of 2D-COS technology in MPs analysis will be discussed. Further, the development and application trends are prospected in microplastic research. With the continuous development of 2D-COS technology, its application in microplastic research should be broad and attractive.

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Oral (L21)

HIGH-RESOLUTION MASS SPECTROMETRY BASED METABOLOMICS FOR DISEASE BIOMARKERS SEARCHING

Ying Liu, Jiang Zhou
Beijing National Laboratory for Molecular Sciences (BNLMS), Analytical Instrumentation Center, College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, China)

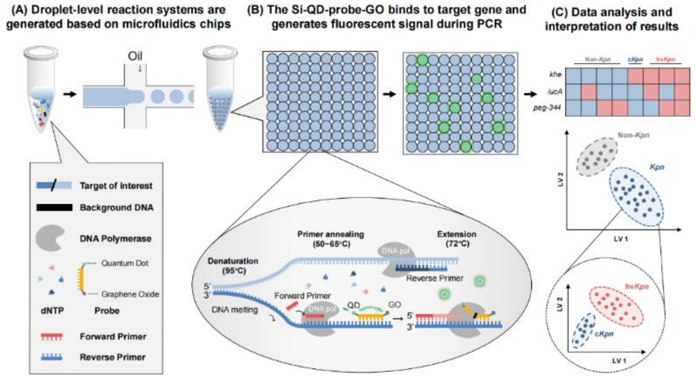
With the rapid development of mass spectrometry (MS) technology, the improvement of resolution provides a foundation for "omics" methods. The use of these techniques helps the discovery of new chemical molecules and biological pathways, continuously updating people's understanding of the mechanisms of life. However, there are still critical problems that need to be improved, such as coverage, reproducibility, and qualitative accuracy in metabolomics and separation efficiency and methods for deconvolution to obtain precise molecular structures. This work focuses on the technical challenges in metabolomics, especially several recent results of new biomarkers for early embryo implantation potential and ovarian cancer ascites' immuno functions.

Oral (L22)

Absolute Quantification of Hypervirulent Klebsiella pneumoniae using Silicon-Doped Carbon Quantum Dot-Probe-Graphene Oxide Nanosensors Combined with Droplet Digital PCR

Lijuan Huang, Bing Du, Xiaohu Cui, Jing Yuan*
Department of Bacteriology, Capital Institute of Pediatrics, Beijing, China

Hypervirulent *Klebsiella pneumoniae* (*hvKp*) poses a severe threat even to healthy individuals, necessitating rapid and accurate detection. Traditional diagnosis relies on TaqMan probe-based qPCR, which suffers from high cost and instability. We developed a novel detection system using a silicon-doped carbon quantum dot (Si-QD)-probe complex immobilized on single-layer graphene oxide (GO) nanosheets. The Si-QD-probe-GO sensor specifically targets virulence genes *khe*, *peg-344*, and *iucA*. This system was integrated with microfluidics-enabled droplet digital PCR (ddPCR) to achieve absolute quantification.The Si-QD-probe-GO complex demonstrated excellent stability at room temperature, minimal photobleaching, and exceptional sensitivity with a detection limit as low as 5 CFU. Quantitative results from ddPCR showed a significant correlation with conventional culture methods ($P < 0.001$). A Partial Least Squares Discriminant Analysis (PLS-DA) model, utilizing the sensor array data, achieved 100% accuracy in distinguishing classical *Klebsiella pneumoniae* (*cKp*) from *hvKp* strains, both in aqueous solutions and infected mouse lung tissue. Validation in a murine pneumonia model confirmed the system's ability to accurately identify *hvKp* in lung tissue, with observed pathological changes aligning with expectations.This study presents a cost-effective, highly stable Si-QD-probe-GO/ddPCR platform for the precise detection and absolute quantification of *Klebsiella pneumoniae*, coupled with reliable virulence determination. Its high sensitivity, specificity, and potential for broad application to other pathogens offer a promising direction for clinical diagnostics.



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Oral (L23)

PROBING THE PHYSICS OF NANOPARTICLES SELF-ASSEMBLY WITH 2D CORRELATION SPECTROSCOPY, TEM AND ELECTRON DIFFRACTION

Biljana Pejova[1], Arej Eid[2,3], Leonardo Lari[2,4], Adam Kerrigan[4], Vlado K Lazarov[2,4] and Ljupcho Pejov[1]

[1]Institute of Chemistry, Faculty of Natural Sciences and Mathematics, SS. Cyril and Methodius University, POB 162, 1000 Skopje, Macedonia
[2] School of Physics Engineering and Technology, University of York, York, UK
[3] University of Tabuk, Tabuk, Saudi Arabia,
[4] The York-JEOL Nanocentre, University of York, York, UK

We demonstrate that by utilization of the state of the art diffraction, imaging and spectroscopic techniques in conjunction with two-dimensional correlation analysis, novel in-depth insights into the physics and chemistry behind the different tendencies towards self-assembling in NiO nanoparticles as function of their surface facets could be provided [1]. Temperature dependent spectroscopic behavior of the two types of NiO NPs, polar versus non-polar faceted is demonstrated to be notably different. Analysis of temperature-dependent spectroscopy data for NiO NPs obtained by the ammonia route with different 2DCOS techniques has revealed that high amount of water molecules that take part in hydrogen-bonding interaction with the surface-adsorbed non-dissociated water molecules on the neutral (100) planes are lost during the thermal treatment and attached back upon cooling. Interactions between water molecules adsorbed on two vicinal NiO NPs are responsible for keeping the self-assembly of the $Ni(OH)_2$ NPs upon heat treatment, as proven by electron diffraction and TEM imaging techniques. In the case of carbamide-based NiO NPs, the self-assembly of initially formed $Ni_3(OH)_4(NO_3)_2$ NPs is not preserved. As revealed by 2DCOS analysis of temperature-dependent spectroscopy data, these NPs are terminated with polar (111) atomic planes, on which water molecules dissociatively adsorb, giving surface hydroxyl groups. The hydrogen bonding proton – donating and accepting abilities are negligible at OH-polar terminated NiO NPs, so that only unfavorable inter-NP interactions are possible, leading to disruption of the NP assembly, which has been shown to take place with transmission electron microscopy and electron diffraction techniques.

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Oral (L24)

WOOD STRUCTURAL FEATURES EVALUATED BY INFRARED SPECTROSCOPY AND 2D-COS

Carmen-Mihaela Popescu, Maria-Cristina Popescu
Petru Poni Institute of Macromolecular Chemistry of the Romanian Academy, 41A Grigore Ghica Voda Alley, RO700487, Iasi, Romania

Wood is a natural material used in large variety of applications due to its properties, abundance, attractive appearance and easy processability. On the other side, due to its structure, wood is susceptible to degradation in the surrounding environment under the action of temperature, humidity, and biological agents. In order to identify the structural changes that occur during natural wood degradation different tratments can be applied.

Here we will present an overview of different thermal treatments applied to wood. These may include the exposure of wooden material for different periods of time at elevated temperatures in dry or wet conditions (variation of temperature – 140, 130, 120 and 110 ^{o}C, variation of relative humidity – 0, 60, 75, 100 %, variation of time – 0 days to 130 days).

For the analysis of these changes and the quantification of the differences between non degraded and degraded wood structure the infrared (FT-IR) spectroscopy, principal component analysis (PCA) and two dimensional correlation spectroscopy (2D-COS) were employed.

Following this, the changes were reflected in shifting of the bands position, modifications in bands intensities and width. Larger variations were observed for the samples exposed at higher temperature values, higher relative humidity values or for longer period.

PCA and 2D-COS analysis made possible to discriminate the changes in the wood structure according to treatment time, amount of relative humidity, or period of exposure, as well as to identify the sequential order of the bands’ modification.

Structural changes identified by infrared spectroscopy could be further corelated with nondestructive mechanical analysis.

Oral (L25)

TWO-DIMENSIONAL INFRARED CORRELATION SPECTROSCOPY STUDYON TWO KINDS OF HYDROGEN-BONDING NETWORKS IN IONIC SOLUTIONS

Daitaro Ishikawa[a]*, Anqi He*[b]*, Yizhuang Xu*[b]*, Tomoyuki Fujii*[a]*, and Yukihiro Ozaki*[c]

[a]*Graduate School of Agricultural Science, Tohoku University, 468-1, Aramaki Aza Aoba, Aobaku, Sendai, Miyagi 980-8572, Japan.* [b]*Beijing National Laboratory for Molecular Sciences, State Key Laboratory for Rare Earth Materials Chemistry and Applications, College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, P. R. China* [c]*School of Biological and Environmental Sciences, Kwansei Gakuin University, Sanda, Hyogo 669 - 1330, Japan*

IR spectra in the 4000-100 cm^{-1} were recorded for four kinds of alkali chloride solutions (LiCl, NaCl, KCl, CsCl solutions) with different concentrations. Two bands were clearly recognized around 3400 and 3160 cm^{-1} in the second derivative spectra; they are assigned to the OH stretching mode of weakly hydrogen-bonded (WHB) and strongly hydrogen-bonded (SHB) water species, respectively. Two-dimensional correlation spectroscopy (2D-COS) was applied to analyze the IR spectra, and it was found that two autopeaks in a 2D synchronous spectrum correspond to the WHB and SHB bands, respectively. Figure 1 shows heterogeneous 2D synchronous correlation spectra between the 4000-3000 cm^{-1} region and the 1000-100 cm^{-1} region illustrating concentration-dependent characteristics of alkali chloride solutions: (A) LiCl, (B) NaCl, (C) KCl, and (D) CsCl. 2D-COS confirmed the existence of two bands around 700 and 350 cm^{-1} in the 1000-100 cm^{-1} region. The bands at 700 and 350 cm^{-1} are due to liberational L2 modes and correlated with SHB (~3160 cm^{-1}) and WHB band (~3400 cm^{-1}), respectively, revealed by the hetero 2D-COS spectrum (Figure 1) . These results suggest the two kinds of hydrogen-bonding networks are constructed by SHB or WHB water species in the alkali chloride solutions.

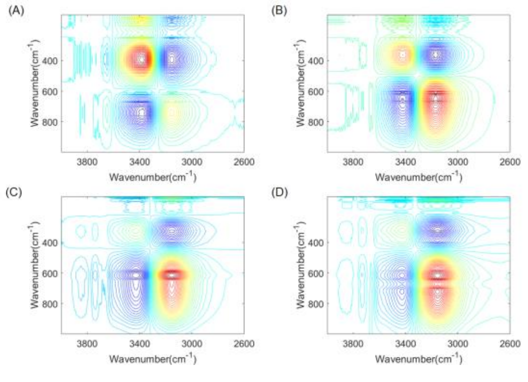

Fig. 1 Heterogeneous two-dimensional synchronous correlation spectra between the 4000-3000 cm^{-1} region and the 1000-100 cm^{-1} region illustrating concentration-dependent characteristics of alkali chloride solutions: (A) LiCl, (B) NaCl, (C) KCl, and (D) CsCl.

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Oral (L26)

Site-Specific Assessment of the Structure and Dynamics of Proteins via Two-Dimensional Infrared Spectroscopy

Feng Gai
College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, China

The infrared (IR) spectrum of a molecule encodes information about its structure and dynamics. However, for complex macromolecules like proteins, it is often difficult, if not impossible, to directly extract site-specific information of interest from their IR spectra, mainly due to spectral overlap and vibrational coupling. A strategy that can help overcome this limitation is to employ external IR probes that bear unique and desired vibrational properties. In this talk, we will discuss how unnatural amino acid-based IR probes can be used in this regard and, through several examples, showcase the utility of several such probes in the site-specific study of the structure, dynamics and interactions of proteins via linear and nonlinear IR spectroscopic techniques.

Oral (L27)

CONVOLUTIONAL AUTOENCODER-BASED FEATURE EXTRACTION FROM AN ENTIRE TWO-TRACE TWO-DIMENSIONAL CORRELATION MAP TO ENHANCE VIBRATIONAL SPECTROSCOPIC DISCRIMINANT ANALYSIS

Seongsoo Jeong and Hoeil Chung

Department of Chemistry, Hanyang University, 222 Wangsimni-ro, Seoul, Republic of Korea

Convolutional autoencoder (CAE)-based feature extraction from entire two-trace twodimensional (2T2D) correlation maps was stuided as a potential tool to enhance the accuracy of vibrational spectroscopybased discriminant analysis. As known, 2T2D correlation maps constructed using only a pair of spectra were effective to highlight minute spectral differences. However, there was an excessive number of features (variables) in 2T2D correlation maps. Therefore, only slice spectra at a wavenumber chosen from the map were typically used for discriminant analysis. In this case, exclusion of a huge number of remaining 2T2D features that would be complementary and descriptive for a given analysis was a major drawback limiting accuracy. Therefore, CAE was adopted to extract features from entire 2T2D correlation maps while minimizing information loss. For evaluation, near-infrared (NIR) and Raman spectra of chili pepper samples and NIR spectra of perilla seed samples were employed for hetero- and homospectral 2T2D correlation analysis, respectively. Then, CAE-extracted features from the 2T2D correlation maps were used to discriminate the geographical origins of samples using support vector machine (SVM). Accuracy was improved by employing CAE-extracted variables in both cases compared with those using slice spectra chosen from the 2T2D maps. Moreover, to provide clearer insight into the models, gradient-weighted class activation mapping (Grad-CAM) identifying the variables significantly contributed to the discrimination was employed in parallel.

Oral (L28)

Toward an in-depth analysis of solid-liquid interface interactions for compounds with potential relevance in bone regeneration and cancer therapy

Edyta Proniewicz

Faculty of Foundry Engineering, AGH University, Reymonta 23 Str., 30-059 Krakow, Poland

One significant challenge in the diagnosing and treating of various diseases, including carcinogenesis, is detecting unlabeled neurotransmitters that mediate the action of metabotropic seven-transmembrane receptors from the G protein-coupled receptor (GPCR) superfamily. Studies have shown that, neurotransmitters play a pivotal role in the development of tumor by stimulating cell proliferation, progression, and metastasis after binding to GPCRs [1]. Consequently, many malignant tumors exhibit elevated GPCR expression on their surfaces [2]. Tumors, particularly those originating in the breast, prostate, thyroid, lungs, and kidneys, often metastasize to bones due to these tissues' unique microenvironment [3]. These receptors have the potential to serve as promising tumor markers, thereby facilitating early treatment and diagnosis, and enabling the assessment of changes in their expression levels. Implementing sensing techniques and therapeutic interventions (pharmaceuticals) that utilize synthetic antagonists and agonists of these receptors can help achieve these ogoals.

Surface-enhanced Raman spectroscopy (SERS) in conjunction with two-dimensional correlation spectroscopy (2DCOS) has emerged as a highly promising method for the biosensing and bioimaging of naurotransmitters and other important biomolecules. This report presents an example of use these methods for an in-depth analysis of:

1) potential-dependent changes in the adsorption of neuromedin C immobilized on an electrochemically roughened silver (AgORC), gold (AuORC), and copper (CuORC) surfaces,
2) L-/D- configuration-dependent changes for neurotensin analog deposited on AgORC, and
3) time-dependent changes for pyridine $\alpha-$aminophosphinic acid on CuO nanostructures.

This work was supported by the National Science Center in Poland (Grant No. 2023/49/B/ST4/00077 and AGH University (Subsidy no. 16.16.170.654).

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Oral (L29)

Insights into Ethanol-water Clusters in Alcoholic Beverages by Spectral Characterizations Connecting with Quality and Taste

Cheng-Feng Zhang[1], Hui-Shuang Li[1], Yi Li[2], Yuqing Wu[1*]
[1]*State Key Laboratory of Supramolecular Structure and Materials, College of Chemistry, Jilin University, No. 2699 Qianjin Street, Changchun 130012, PR China;* [2]*China Light Industry Enterprises Investment and Development Association, 22B. Fuwai Avenue, Xicheng District, Beijing 100833, PR China*

The quality and taste of alcoholic beverages are influenced not only by the types and concentrations of involved components but also by the supramolecular clusters of ethanol-water (E-Wc). The intrinsic hydrogen bonds (HBs) within these clusters are closely related to sensory experience and quality evaluation, and their structural characteristics and dynamic behaviors are gradually being revealed. However, current understanding of E-Wc, particularly their intrinsic relationship with the sensory attributes of beverages, still lacks systematic clarification. To gain deeper insights into the driving mechanisms of these clusters in alcoholic beverages, this article summarizes studies employing various spectroscopic techniques, including fluorescence emission, nuclear magnetic resonance (NMR), infrared/near-infrared absorption spectroscopy, and Raman scattering, to investigate supramolecular E-Wc in alcoholic beverages. Among them, two-dimensional correlation analysis (2D-COS) has been widely applied as a powerful tool for deciphering the key structural features of these clusters. With the help of carving important supramolecular E-Wc, hopefully the prospects and challenges in this field will be clearer and more modulated products with various tastes and quality will be developed in the alcoholic industry.

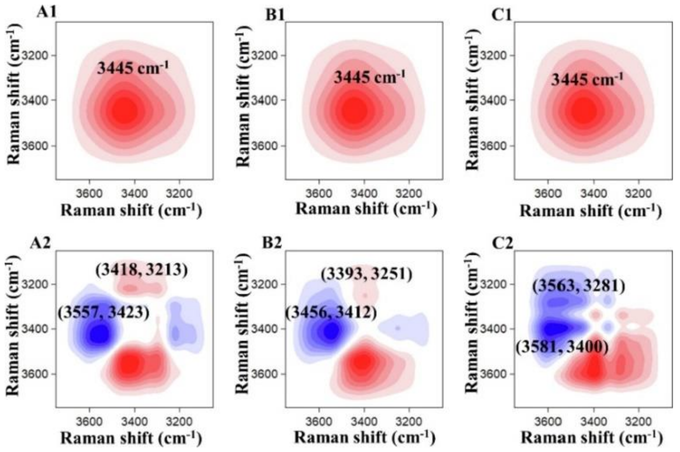

Figure 1. (A1-C1) Synchronous and (A2-C2) asynchronous 2D-COS of *Fenjiu* (a) measured over incubation times for (A) 1-hour, (B) 3-day, and (C) 7-day. The blue and red area denote negative and positive sign, respectively.

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Oral (L30)

TRIBOELECTRIC SPECTROSCOPY AND DEEP LEARNING FOR LIQUID SENSING

Hongyan Dai, Yang Li, Shiyu Wang, Yutong Wang, Jun Dong, Gang Ma*
Key Laboratory of Medicinal Chemistry and Molecular Diagnosis of Ministry of Education, Key Laboratory of Analytical Science and Technology of Hebei Province, State Key Laboratory of New Pharmaceutical Preparations and Excipients, College of Chemistry and Materials Science, Hebei University, Baoding 071002, China

Sensing, the process of detecting and measuring physical, chemical, or biological signals, is a fundamental pillar of modern technological advancements. Among the various types of sensing technologies, liquid sensing plays a crucial role in applications such as environmental monitoring, healthcare diagnostics, and industrial process control. Recently, solid-liquid triboelectric nanogenerators (SL-TENGs) have garnered increasing attention as a promising technology in the field of liquid sensing.[1-4] The working principle of SL-TENGs is based on the coupling effect of triboelectrification and electrostatic induction, which converts mechanical energy into electrical energy.[4-9] SL-TENGs not only efficiently harvest high-entropy water energy from the environment, but also exhibit a specific response to changes in solution concentration and composition. By utilizing the concept of triboelectric spectroscopy,[2] SL-TENGs offers unique advantages in liquid sensing. In light of this, the present study will report on the applications of SL-TENGs in sensing inorganic systems, organic systems, food systems, and biological systems. Additionally, it will also highlight our research progress in integrating deep learning techniques with SL-TENGs for enhanced sensing capabilities.

* Corresponding author (gangma@hbu.edu.cn)

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Oral (L31)

APPLICATION OF DEEP-LEARNING TO PROBE SUBTLE SPECTRAL VARIATION CAUSED BY INTERMOLECULAR INTERACTIONS

Guanlin Lu[1] Shiliang Zhang[2] Yizhuang Xu[3]

[1]*School of Electronic and Computer Engineering, Peking University Shenzhen Graduate School, Shenzhen 518055, China*
[2]*School of Computer Science, Peking University, Beijing 100871, China*
[3]*College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, China*

Intermolecular interactions play a critical role in the construction of supramolecular systems[2], and two-dimensional correlation spectroscopy has become an important tool in the characterization of intermolecular interactions[3]. Our previous researches have demonstrated that subtle changes on peak position, peak width, and peak intensity caused by the intermolecular interaction can be revealed from the characteristic pattern of cross peaks in the corresponding 2D asynchronous spectrum constructed by the DAOSD approach[1]. However, the pattern of cross peaks in the 2D asynchronous spectrum become too complex to reflect the detailed spectral variation as multiple supramolecular aggregated are generated via the interaction.

To address this challenge, we propose a deep-learning-based approach to model the complex mapping between the pattern of cross peaks in the 2D asynchronous spectra and the spectral variation brought about by the interaction. In the same solutions, two solutes (P and Q) are present. Two supramolecular aggregates (PQ and PQ_2) are produced via the interaction between P and Q, we generated a dataset of 1.1 million pairs of 2D asynchronous spectra matrices. The model inputs include both the original matrix data and geometric features such as curvature, gradient, and direction extracted from Hessian matrices to capture contour-like structures in the spectra. We evaluated several backbone networks—ResNet18, ResNet34, ResNet50, ResNet101, and ResNet152—and achieved mean errors of 0.2032, 0.1874, 0.1463, 0.1330, and 0.1369 nm, respectively, after applying active learning and regional fine-tuning. Via this network, the spectral feature of PQ and PQ_2 can be faithfully predicted from the given patterns of cross peaks from a pair of 2D synchronous spectra generated via the DAOSD approach[1]. The approach descried in the present work provides a chance to get insight into the physiochemical nature of intermolecular interaction in many complex systems.

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Oral (L32)

INVESTIGATION OF *SCUTELLARIA BAICALENSIS* ROOTS USING 2T2D CORRELATION FTIR SPECTROSCOPY

Bogumiła Kupcewicz[1], Agata Świątły-Błaszkiewicz[1], Jakub Gębalski[2], Daniel Załuski[2]
[1]Department of Inorganic and Analytical Chemistry, Collegium Medicum in Bydgoszcz, Nicolaus University in Toruń, Poland
[2]Department of Pharmaceutical Botany and Pharmacognosy, Collegium Medicum in Bydgoszcz, Nicolaus University in Toruń, Poland

Scutellaria baicalensis (SB) is a medicinal plant with notable pharmacological properties. Its roots are rich in bioactive compounds like flavonoids, diterpenes, iridoids, and polysaccharides that offer potential therapeutic benefits. In our study, *SB* roots were collected in three seasons (spring, summer, and autumn) and dried at room temperature or lyophilized (freeze-dried). The dried roots were then extracted using three techniques: maceration, reflux extraction, or ultrasound-assisted extraction with 75% methanol as the solvent [1].

In this study, we explore using two-trace two-dimensional (2T2D) correlation spectroscopy based on ATR-FTIR spectra for analysing variations in the composition of samples due to different harvesting seasons, drying, and extraction conditions. Preliminary findings have been recently published [1]. To extend our study, the various approaches for analysing and interpreting synchronous and asynchronous 2T2D correlation spectra were used and compared [2,3]. We have focused on the identification of flavonoids, particularly baicalin and baicalein, which are the primary active compounds within the plant material, as well as monitoring of their variations. Additionally, various chemometric methods were employed to assess their effectiveness in discriminating samples according to harvest season, drying method, and extraction technique. The chemometric methods were applied to both raw and pre-processed ATR-FTIR spectra, along with 2T2D correlation maps and slices.

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Oral (L33)

RAPID QUANTITATIVE ANALYSIS OF NITROGEN AND PHOSPHORUS IN DAIRY COW MANURE BASED ON NEAR INFRARED SPECTROSCOPY AND DEEP LEARNING

Qiao-Lin Zhang[1],*Gui-Mei Dong*[1]*,*Ren-Jie Yang*[1]， *Run Zhao*[2]*, *Zeng-Jun Yang*[2],
[1]College of Engineering and Technology, Tianjin Agricultural University, Tianjin, 300384
[2]Agro-Environmental Protection Institute, Ministry of Agriculture and Rural Affairs, Tianjin 300191, China
**guimeidong@gmail.com* **zhaorun@aepi.org.cn*

Nitrogen and phosphorus are important indicators for the scientific return of manure water to the fields in large-scale dairy farms. Rapid and accurate determination of nitrogen and phosphorus content in manure water is the primary problem that dairy farms need to solve on the road of combining farming and breeding at this stage. This paper combines near-infrared spectroscopy (NIRS) with a variety of modeling algorithms to explore the feasibility and modeling strategy of NIRS in the quantitative analysis of nitrogen and phosphorus in dairy cow manure water. By comparing the differences in modeling accuracy and generalization ability between traditional modeling methods and machine learning algorithms and deep learning algorithms, the importance of the complexity of manure water composition to the selection of modeling methods is revealed. The results show that the deep learning model performs best in processing complex spectral data of manure water, and its prediction accuracy is significantly better than that of traditional modeling algorithms and machine learning algorithms, and it has high application potential. This study provides technical support for the precise management and scientific return of manure water nutrients to the fields in large-scale dairy farms.

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Oral (L34)

APPLICATION OF TWO-DIMENSIONAL CORRELATION SPECTROSCOPY IN MONITORING EMERGING INTERACTIONS BETWEEN QUINIDINE AND SELECTED d-ELECTRON METALS

Zofia Chajdaś, Martyna Kucharska, Aleksandra Wesełucha-Birczyńska,
Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387 Kraków, Poland

The purpose of this work was to monitor the crystallization process of quinidine compounds, an alkaloid with antimalarial properties, with Cu(II) and Cd(II)[1]. UV-Vis and Raman spectroscopy measurements were carried out and then analyzed by 2D-COS spectroscopy in Omnic v.9.3 SpectraCorr software regarding time of crystallization as a perturbation. As a result, it was possible to observe shifts in the bands, resulting from the formation of interactions between the quinoline alkaloid and metals (Fig.1).

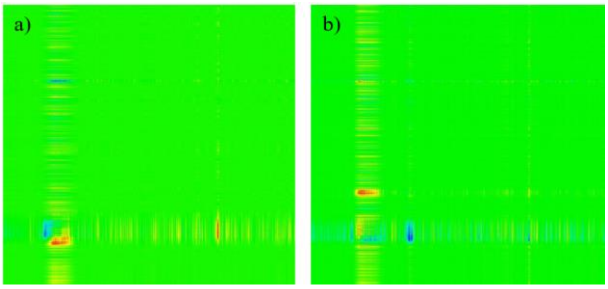

Figure 1. Asynchronous spectra of Cu(II)-Qd (a) and Cd(II)-Qd (b), obtained from Raman spectroscopy

In the 2D-COS Raman asynchronous spectra, changes were marked by cross-peaks at +(1018, 3354), +(1212, 3370), +(1387, 3365), +(1430, 3365), -(1599, 3365), +(1643, 3369) cm^{-1} for Cu(II)-Qd and +(1331, 3348), +(1358, 3363), +(1388, 3495), +(1388, 2780), -(1388, 3405), +(1593, 3354) cm^{-1} for Cd(II)-Qd.

In the 2D-COS UV-Vis asynchronous spectra, shifts in bands were marked by cross-peaks at +(207, 232), +(251, 234), +(253, 206) nm for Cu(II)-Qd and -(209, 237), +(234, 250), +(236, 207), -(249, 234) nm for Cd(II)-Qd.

The above results indicate the formation of interactions between quinoline/quinuclidine rings of quinidine and metal ions[2].

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Oral (L35)

COMPETITIVE CO-EXISTING POLYCYCLIC AROMATIC HYDROCARBONS ADSORPTION ON AGED POLYVINYL CHLORIDE MICROPLASTICS: TWO-DIMENSIONAL CORRELATION SPECTROSCOPY STUDY

Jia Long, Yi-yang Qing, Ren-Jie Yang*, Ji-yuan He, Gui-Mei Dong, Fan Yang
College of Engineering and Technology, Tianjin Agricultural University, Tianjin, 300384
*rjyang1978@163.com

The natural aging of microplastics (MPs) in the real environment with competitive adsorption of multiple coexisting polycyclic aromatic hydrocarbons (PAHs) significantly increases the risk of contamination. In this study, we examined the preferential adsorption behavior of naphthalene (NAP), phenanthrene (PHE), and benzo[ghi]perylene on aged polyvinyl chloride (PVC), through adsorption kinetics and isotherm experiments. Fourier transform infrared (FTIR) spectra revealed that adsorption did not result in the formation of new chemical bonds. Two-dimensional correlation spectroscopy (2D-COS) revealed that the co-existence of hydrophobic interaction, electrostatic interaction and π-π stacking in competitive adsorption, which interfered with the hydrophobic-dominated adsorption mode, weakened the PAHs' C-H bond binding, prompted the C-Cl bond to take the lead in the response. The present study confirms that FTIR coupled with 2D-COS is an effective means to analyse the microscopic interaction mechanism of MPs-pollutants in complex environments.

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Oral (L36)

Assessing Compost Maturity Dynamics: Unraveling Dissolved Organic Matter Signatures using EEM-PARAFAC and 2D-COS

Xi Li[1], Wen-Jiao Qin[2], Ren-Jie Yang[1]*, Gui-Mei Dong[2],
Run Zhao[2], Zeng-Jun Yang[2]*
[1]College of Engineering and Technology, Tianjin Agricultural University, Tianjin, 300384
[2]Agro-Environmental Protection Institute, Ministry of Agriculture and Rural Affairs, Tianjin 300191, China
*rjyang1978@163.com, yangzengjun@caas.cn

Aerobic composting, as a key resource-based technology, still faces challenges in improving its maturity assessment system. In this study, the evolution of dissolved organic matter (DOM) was investigated using Excitation Emission Matrix (EEM) and two-dimensional correlation spectroscopy (2D-COS) to elucidate correlations of DOM humification and maturity and structural dynamics. The results showed that the humification process of DOM could be quantified using fluorescence spectral index as shown in Fig. 1, and its structural evolution was closely related to the maturity of the compost. Fig.2 showed the presence of automatic peaks at 1627, 1500, 1329, 1168, 1055 and 910 cm^{-1}, indicating that polysaccharides, aliphatics and aromatics changed most significantly during the composting process. Combined with the key physicochemical indicators, it was demonstrated that the accumulation of humic acids was closely related to the reduction of C/N and EC values. These findings provide a theoretical basis for rapid assessment of maturity, leading to optimization of composting parameters and real-time monitoring.

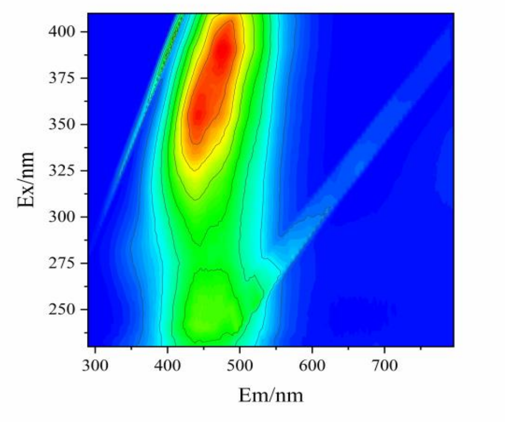

Figure 1. EEM spectrum of DOM

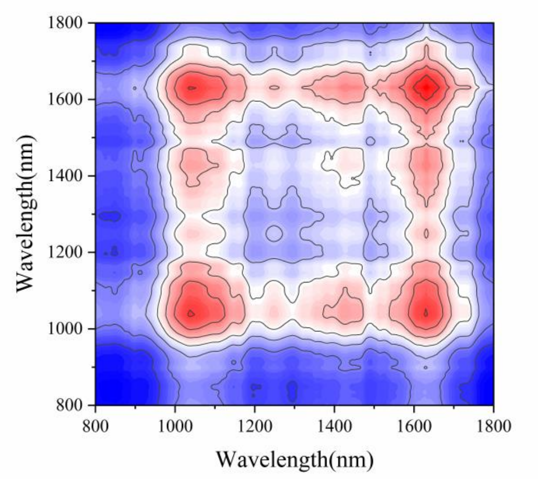

Figure 2. Synchronous two-dimensional correlation spectrum of DOM

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Oral (L37)

TIME-RESOLVED IR DIFFERENCE SPECTROSCOPY COUPLED TO 2D-COS ANALYSIS : APPLICATIONS TO THE STUDY OF THE MECHANISM OF PHOTOSYNTHETIC REACTIONS

Alberto Mezzetti[1,2], Winfried Leibl[2], Elizaveta Grishaeva, Marco Malferrari[3], Giovanni Venturoli[4], Francesco Francia[4], Isao Noda[5]
1 Sorbonne Université, CNRS, Laboratoire de Réactivité de Surface (LRS), Paris, France
2 Institute for Integrative Biology of the Cell (I2BC), CEA, CNRS, Université Paris-Saclay, France
3 Dipartimento di Chimica “Giacomo Ciamician”, Università di Bologna, Bologna, Italy
4 Laboratorio di Biochimica e Biofisica Molecolare, Dipartimento di Farmacia e Biotecnologie, FaBiT, Università di Bologna, Bologna, Italy
5 Department of Materials Science and Engineering, University of Delaware, Newark, DE, USA

Time-resolved IR difference spectroscopy is a widely used technique in biochemistry to investigate, at an atomic level, the mechanism of biochemical reactions. It is particularly well-suited to study light-induced reaction, and is therefore not surprising that it has been widely applied to photosynthesis in the last 35 years.

The use of 2D-COS to intepret IR difference spectra is however still quite limited, especially in photosynthesis, mainly for historical reasons (some pioneers of time-resolved IR difference spectroscopy were among the developers of chemometric strategies for global fitting of band kinetics).

We have applied 2D-COS to analyze data reflecting photoinduced charge separation and dark recombination in the photosynthetic reaction center of the bacterium R. sphaeroides [1].

Two different illumination schemes were adopted. Whereas the use of a laser flash (duration: 7 ns) made it possible to follow the kinetics of recombination of the light-induced state P+A- to the neutral state PA, the use of a 20.5 s continuous light from a lamp made it possible to follow both the build-up of a steady-state P+A- population and its decay to PA.

Comparison between P+ A- /PA IR difference spectra obtained under (or 650 ms after) continuous illumination and obtained after one laser flash show small but meaningful differences, reflecting structural changes in the light-adapted state produced by continuous illumination. These differences are very similar to those we observed when comparing IR difference spectra reflecting charge separation in photosystem II (the water oxidizing enzyme) in light-adapted states and non-light-adapted states [2]).

Two-dimensional correlation spectroscopy analysis revealed that in all the observed series of time-resolved IR difference spectra (under illumination, after illumination, and after laser flash), marker bands at 1749, 1716, and 1668 cm^{-1} all evolve synchronously, demonstrating that electron transfer reactions and protein backbone response (at least the one reflected by the 1668 cm^{-1} band) are strongly correlated. Conversely, for spectra under and after continuous illumination, many asynchronicities are observed for (still unassigned) bands throughout the whole 1740–1200 cm^{-1} region, reflecting a more complicated molecular scenario in the RC upon build-up of the light-adapted state and during its relaxation to the resting neutral state.

We have recently extended the use of 2D-COS to analyze time-resolved IR difference spectra reflecting the photoativation of the Orange carotenoid Protein, involved in the photoprotection of cyanobacterial photosynthetic apparatus. Preliminary results of this analysis wil also be presented.

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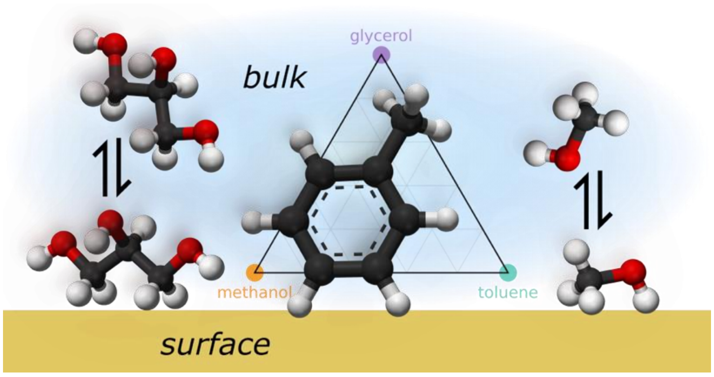
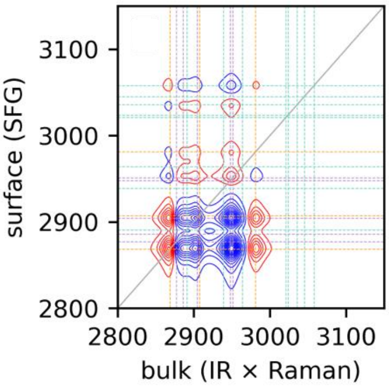
Oral (L38)

Surface–Bulk Heterospectral Correlation Spectroscopy to Characterize the Adsorption of Molecules from Ternary Mixtures onto Solid Surfaces

Dennis Hore and Mahsa Torkamanasadi
Department of Chemistry, University of Victoria
Victoria, British Columbia, Canada

The adsorption of molecules onto surfaces from the bulk liquid phase is a critical feature of industrial and biological fouling, the compatibility of materials for medical implants, and a host of environmental processes on mineral surfaces. Surfaces have a unique ability to concentrate adsorbates due to favorable surface interactions. As a result, the reactive of molecules on surfaces may be substantially enhanced with respect to bulk liquid or aqueous phases. It is therefore of interest to determine the surface preference of a particular adsorbate. Vibrational sum-frequency generation has the advantage of being a label-free technique on account of its intrinsic molecular specificity and can isolate contributions from surfaces due its symmetry-breaking requirement as a second-order nonlinear optical phenomenon. We have previously illustrated how this technique may be used in combination with IR absorption and/or Raman scattering to determine the surface excess for a binary mixture.[1–5] In the case of 3-component mixtures, the situation is slightly more complicated as the nature/direction of the concentration perturbation must be selected.[6] We illustrate a method for this, along with an associated set of rules for interpreting the sign of heterospectral surface-bulk cross peaks for ternary mixtures.





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Oral (L39)

Structures of Gas-Phase Large Molecular Clusters Studied by Two-Dimensional Correlation IR Spectroscopy

Yoshiteru Matsumoto

Department of Chemistry, Faculty of Science, Shizuoka University, Ohya 836, Suruga, Shizuoka 422-8529, Japan

A large molecular cluster comprising approximately 100 molecules represents an intermediate state between gas-phase small clusters and bulk materials. Such clusters possess an internal core resembling that of the bulk phase, surrounded by an external surface directly exposed to vacuum. Owing to this unique structure, the surface exhibits properties analogous to small gas-phase clusters, while the core behaves more like bulk matter. As a result, large molecular clusters are of significant interest as hybrid systems with physicochemical characteristics markedly distinct from those of bulk materials.

Infrared (IR) spectroscopy serves as a powerful probe for elucidating the intermolecular structures of such clusters, with vibrational signatures offering detailed insight into the evolution of hydrogen bonding as a function of cluster size. However, large molecular clusters often display broad spectral features due to band overlap, reminiscent of bulk liquids and solids. To resolve these complex spectral profiles, mathematical decomposition techniques must be applied to isolate individual vibrational bands. Subsequently, two-dimensional correlation spectroscopy (2D-COS) is employed on the IR absorption spectra acquired via IR cavity ringdown spectroscopy.

We first examine acetylene clusters, wherein CH stretching vibrations were observed under varying sample gas concentrations in a supersonic jet.[1] 2D-COS analysis reveals that the broad IR signature decomposes into two distinct CH stretches, corresponding to pure and polycrystalline orthorhombic phases present within aerosol particles.

Secondly, we investigate the CH stretching Fermi triad in benzene clusters. 2D-COS unveils that the triad consists of two series of bands. Through molecular dynamics simulations combined with electronic state theory, we tentatively attribute these bands to CH stretches originating from surface and core molecules within the large benzene clusters.

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Oral (L40)

Adaptive 2T2D spectral feature extraction method for improving the component identification performance in mixtures based on handheld Raman technology

Xin Zhao, Ziyan Zhao, Qibing Zhu, Min Huang

Key Laboratory of Advanced Process Control for Light Industry (Ministry of Education),
School of Internet of Things Engineering, Jiangnan University, Wuxi 214122, P. R. China

Accurate identification of specific components in mixtures is critical in chemical engineering, food safety, and biomedical sciences. Raman spectroscopy provides spectral information based on molecular vibrations, with peaks acting as 'fingerprints' of substances. Its simplicity, speed, and non-destructive nature make it a key tool for mixture analysis [1]. Component identification involves analyzing peak positions, strengths, and shapes. Conventional methods rely on database matching but face challenges such as complex data processing and slow analysis. Deep learning automates feature extraction from large datasets, improving identification and classification [2]. However, detecting low-concentration components remains difficult due to weak signals, noise, and potential peak overlap, exacerbated by the lower precision of handheld devices [3].

To address this, reference spectra of pure substances at low concentrations are introduced into two-trace two-dimensional correlation spectroscopy (2T2D-COS) to highlight its information content. Additionally, deformable convolutions (DCNs) are integrated into the model to capture irregularly shaped peak regions in synchronous 2T2D-COS, improving recognition accuracy. Experiments validate the effectiveness of combining 2T2D-COS with DCN-enhanced deep learning models.

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Oral (L41)

A method for improving the signal intensity and signal-to-noise ratio of two-trace two-dimensional correlation spectroscopy

Linchen Xie [a], *Yizhuang Xu* [b]*, *Kun Huang* [a]*
[a] *School of Metallurgical and Ecological Engineering, University of Science and Technology Beijing, Beijing 100083, China*
[b] *Beijing National Laboratory for Molecular Sciences, State Key Laboratory for Rare Earth Materials Chemistry and Applications, College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, China*

Two-trace two-dimensional correlation spectroscopy (2T2D-COS) has been widely used to investigate interactions in complex mixtures [1]. However, compared to generalized 2D-COS its low signal intensity and poor signal-to-noise ratio (SNR) limit the detection of subtle interactions. In this study, we present a method for enhancing the cross-peak intensity and SNR in 2T2D-COS. First, three simulated 1D spectra were used to generate three 2T2D-COS (denoted as Ψ_1, Ψ_2 and Ψ_3; Fig. 1a-c). By aligning the signs of the Ψ_1-Ψ_3 and summing these cross peaks, we obtain an enhanced 2T2D-COS Ψ_4 (Fig. 1d) that is 10 times stronger than Ψ_1-Ψ_3. Second, we identified a linear correlation ($R^2 = 0.9975$) between cross-peak volume and standard deviation (Fig. 2). Normalization Ψ_1-Ψ_3 by peak volume reduces the standard deviation of Ψ_4 and improves the SNR. This method is expected to improve the sensitivity of detection of weak intermolecular interactions in complex systems.

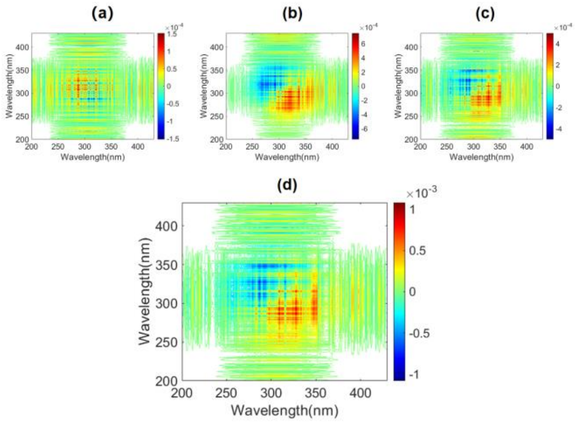

Figure 1. The 2T2D-COS of Ψ_1 (a), Ψ_2 (b), Ψ_3(c) and Ψ_4 (d).

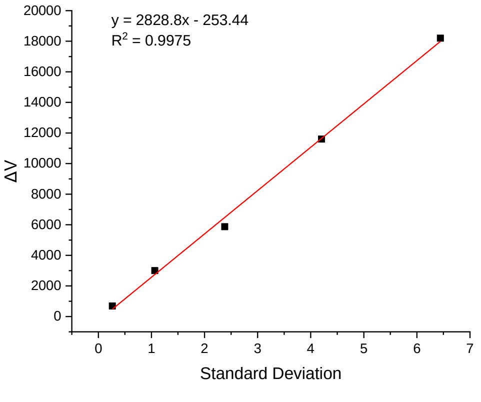

Figure 2. The linear correlation of the peak volumes and standard deviations.

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Oral (L42)

APPLICATION OF THE COMBINATION OF DEEP LEARNING AND TWO-DIMENSIONAL RELATED SPECTRA TO EXPIRED DRINKS

Linyue Dai, Haojiang Zhang, Juan Feng, Hao Lin
School of Life Science and Technology, UESTC, Chengdu, Sichuan

Abstract It is harmful for health to drink expired drinks. Here we utilized the combination of deep learning method and two-dimensional related spectra to try to distinguish if drinks are expired or not. Firstly, fluorescence emission spectra are collected on drinks which are kept different days. Two-dimensional related spectra are then obtained with changing the excitation wavelength. Next, we carried deep learning on two-dimensional synchronous or asynchronous spectra and some results are obtained.

Keywords expired drinks, deep learning, two-dimensional related spectra

Oral (L43)

CONSTRAINTS IN THREE-WAY MULTIVARIATE CURVE RESOLUTION

Xin Zhang[1]*, Roma Tauler*[2]

[1]*Department of Chemistry, Capital Normal University, Beijing, China*
[2]*Institute of Environmental Assessment and Water Research (IDAEA), Consejo Superior Investigaciones Científicas (CSIC), Barcelona, España, Spain*

Multivariate Curve Resolution (MCR) is a matrix decomposition method used to resolve mixture analysis problems and has been employed in chemometrics and various scientific fields for approximately three decades. However, due to the inherent ambiguity of the MCR method, multiple feasible solutions can be generated[1]. Therefore, constraints need to be applied to reduce ambiguity and enhance the interpretability of the results. When the trilinear constraint is applied on the LC-MS or GC-MS data, peak shifts in retention time can lead to incorrect solutions. Therefore, we compared the effects of applying the Flexible Trilinearity Alignment (FTA) and Shift Invariant Transformation (SIT) constraints in MCR-ALS. These were also compared with the traditional trilinear model. The study involved the analysis of both synthetic and experimental datasets, focusing on their effectiveness in handling peak shifts in chromatographic analysis. The FTA and SIT methods performed well in handling chromatographic peak shifts, especially in noisy data, effectively reducing rotational ambiguity[2]. Under certain experimental conditions, the traditional trilinear model may be more suitable, particularly when there are significant changes in the shape of the retention time curves.

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Oral (L45)

PREPARATION AND OPTIMIZATION OF TEMPERATURES FOR ENHANCED FLUORESCENCE OF Na_2WO_4/Eu(TTA)$_3$(TPPO)$_2$ COMPOSITES

Jianguo Chang, *Dongliang Tao*

Anhui Provincial Key Laboratory of Green Carbon Chemistry, School of Chemistry and Material Engineering, Fuyang Normal University, Fuyang 236037, China

Rare-earth metals have great application potential due to their unique luminescence. The "antenna effect" can enhance the luminescence of rare-earth ions by forming complexes between the ions and organic ligands. However, the resulting rare-earth complexes still suffer from drawbacks such as high cost and low quantum yield, which greatly limit their large-scale application.

In this study, the effects of different temperatures on the properties of core-shell fluorescent materials were systematically investigated via the solvothermal method, using low-cost and readily available sodium tungstate (Na_2WO_4) as the core material and rare earth europium complex Eu(TTA)$_3$ (TPPO)$_2$ (TTA is 2-thienoyltrifluoroacetone and TPPO is triphenylphosphine oxide) as the shell. The results showed that the europium complex was successfully coated onto the surface of Sodium Tungstate, the morphology of the composite was uniform, and the surface defects of the core material were effectively passivated by the shell. At 40 ℃, the quantum efficiency of the composites was about 56%, which is 1.3-fold higher than that of the Eu(TTA)$_3$(TPPO)$_2$ (42%).

Our group has been dedicated to designing and synthesizing a novel class of luminescent materials, e.g., Na_2SiO_3/Eu (TTA)$_3$(TPPO)$_2$, $NaAlO_2$/Eu (TTA)$_3$(TPPO)$_2$, Na_2CO_3/Tb (TTA)$_3$(TPPO)$_2$, and $CaCO_3$/ Eu (TTA)$_3$(TPPO)$_2$.These materials overcome the intrinsic limitations of conventional rare-earth complexes (e.g., high cost and low quantum yield) by integrating europium(III) complexes into inorganic matrices. This strategy not only enhances luminescence performance but also establishes a general approach for constructing inorganic-hosted europium(III)-based red-emitting materials, offering new possibilities for applications in optoelectronics and sensing.

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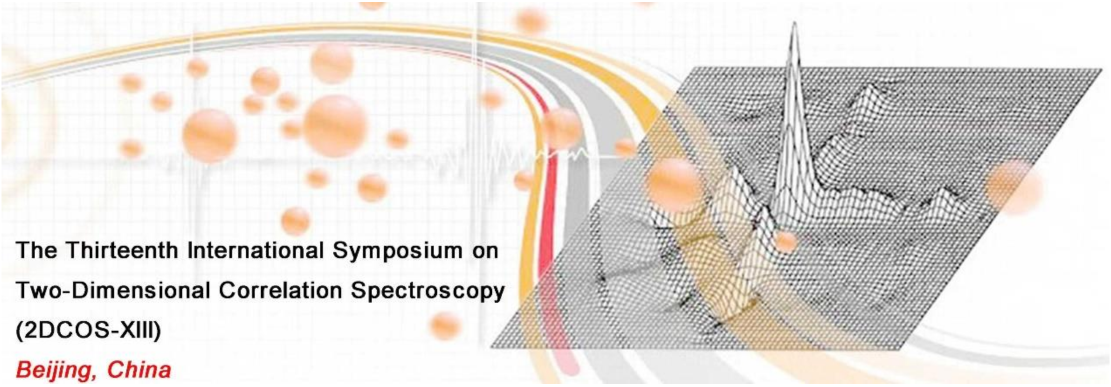
abstracts of posters



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Poster (P1)

2D-COS IN THE ANALYSIS OF SAMPLE PREPARATION METHOD

Emilia Wrona[1], Anna Błasiak[2], Gabriela Stopka[2], Aleksandra Nogaj[2], Aleksandra Kurek[1],
Aleksandra Wesełucha-Birczyńska[1]

[1] *Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387 Kraków, Poland*
[2]*Department of Neurophysiology and Chronobiology, Institute of Zoology and Biomedical Research, Jagiellonian University, Gronostajowa 9, 30-387 Kraków, Poland*

Raman spectroscopy is a non-invasive technique with applications in biomedicine[1]. Analysis of the composition and concentration of lipids in brain tissue can change significantly in diseased tissues, making it a useful diagnostic parameter for determining the type and severity of a brain tumour or neurodegenerative disease. Obtaining high-quality results, however, is difficult due to the appropriate preparation of the tissue and the selection of appropriate measurement parameters[2]. Raman spectroscopy allows measurements to be performed on tissue that has not been previously fixed[3–6]. However, the currently available literature does not provide clear guidance on how to prepare a brain tissue sample to obtain the highest possible spectrum quality.

The objective of the present study was to investigate what effect the temperature at storage of brain tissue from the rat has on the quality of the spectra. Based on the literature review, three methods were selected for the storage of brain tissue[3–6].

Method I: tissue was stored at room temperature immersed in artificial cerebrospinal fluid (ACSF), which was carbogenised.

Method II: the tissue was kept in a container placed on a cooling pads. The tissue was immersed in artificial cerebrospinal fluid, which was carbogenised. The tissue was then transferred to a measuring vessel containing chilled ACSF.

Method III: the tissue, was frozen in liquid nitrogen. Before measurement, the tissue was warmed and then placed in a measuring vessel containing 0.9% saline solution.

The temperature of the ACSF solution was kept constant at 32°C during each measurement. The resulting Raman spectra were pre-processed and averaged. Using SpectraCorr software, a 2T-2D analysis was performed, comparing the spectra obtained by different methods with each other[7]. On the basis of 2D maps, differences were identified and discussed.

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Poster (P2)

2T2D-COS OF RAT BRAIN TISSUE WITH FEATURES OF NEURODEVELOPMENTAL DISORDER

Dominika Matuszyk[1], Anna Błasiak[2], Emilia Wrona[1], Aleksandra Nogaj[2], Aleksandra Kurek[1], Anna Kołodziej[1], Aleksandra Wesełucha-Birczyńska[1]

[1] *Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387 Kraków, Poland*

[2]*Department of Neurophysiology and Chronobiology, Institute of Zoology and Biomedical Research, Jagiellonian University, Kraków, Poland*

Autism spectrum disorders (ASDs) are characterized by complex and heterogeneous symptomatology, and their etiology remains incompletely understood. Certain environmental factors, such as prenatal exposure to valproic acid (VPA), have been shown to increase the risk of neurodevelopmental disorders in offspring. Based on this association, a widely used, validated preclinical rodent model of autism has been developed, reflecting behavioral and neuroanatomical changes characteristic of ASD.[1,2]
The aim of this study was to compare the chemical composition of brain tissue from a VPA-induced ASD rat model with that of a control rats using Raman scattering spectroscopy. Brain samples obtained from approximately 5-week-old Sprague Dawley rats were maintained during the measurements in an incubation chamber ensuring constant conditions of temperature (32 °C), humidity (at approximately 70%), and CO2 concentration (0.1%). Measurements were performed using Renishaw inVia Qontor Raman spectroscope with a 785 nm laser.
Data analysis included spectral averaging, principal component analysis (PCA) and two-trace two-dimensional correlation spectroscopy (2T2D-COS)[3]. The results indicate alterations in the protein and lipid structure of the brain tissue in the VPA-ASD rat model compared to the control group. For example, the cross-peak of 1300 cm^{-1} indicates saturated fatty acids characterizing healthy tissue, and the 1683 cm^{-1} amide I band characterizes the β-conformation of autistic tissue.

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Poster (P3)

Multimodal Models Pork Spectral Recognition Model Based on Cross-Attention

Yu Xue, Jing Liang
College of Artificial Intelligence, Nankai University, Tianjin, 300350, China

Food safety has received increasing attention in recent years, especially for meat products. There have been many incidents that seriously affect public health, such as using spoiled meat to substitute for good, mixing with additives, and so on. Food inspection requires a large amount of manpower and resources, and with the development of artificial intelligence, people are beginning to use computer vision to address such issues. Deep learning can better improve the performance of neural networks in object recognition, Structures such as Transformer[1], ResNet[2] and so on, greatly enhance the performance of network models in recognition tasks.

Vibration spectroscopy detection can quickly and accurately detect targets. Two-dimensional correlation spectroscopy (2D-COS) generates synchronous and asynchronous spectra by analyzing dynamic spectral data. This study will integrate 2D-COS with other modal data (such as mass spectrometry, XRD) to enhance detection robustness through multimodal learning. By utilizing the attention mechanism of Transformer, a cross-attention mechanism was designed to integrate features from two different modalities by inputting 2D-COS images and one-dimensional mass spectrometry vectors. In the design of the decoder, two different decoders, CNN and Transformer, were selected. Convolutional decoders can better restore detailed features, while Transformer decoders can better establish long-range dependencies. Experimental results demonstrate that the proposed method offers notable advantages in terms of low-concentration detection sensitivity.

This method verifies the improvement of recognition performance of 2D-COS by multimodal models. Comparative experiments demonstrate have shown that under noisy conditions, hybrid deep learning architectures outperform traditional chemometric methods by 15-25% in terms of classification accuracy and robustness. The proposed model has shown good performance in detecting mixed meat tasks and has practical significance in food safety applications.

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Poster (P4)

PORIA ADULTERATION DETECTION BASED ON DEEP LEARNING AND NEAR-INFRARED TWO-DIMENSIONAL CORRELATION SPECTROSCOPY

Rongzhen Mao[1], Jing Liang[1], Mingyue Huang[1], Bin Wang[1], Xiaoxuan Xu[1], Mingzhu Yang[2], Lei Liu[1], Jing Xu[1]
1 College of Artificial Intelligence, Nankai University, Tianjin, 300350, China
2 Nankai university hospital, Nankai university, Tianjin, 300350, China

As a traditional Chinese medicinal material, the quality of Poria significantly affects its pharmacological efficacy [1-3]. However, adulteration of Poria cocos in the market has been frequently observed, which not only compromises its medicinal value but also jeopardize people’s health. Traditional adulteration detection methods suffer from low efficiency, high cost, and poor adaptability to complex samples [4-5]. Therefore, a lightweight and efficient convolutional neural network (CNN) model was proposed. The model utilizes preprocessed two-dimensional correlation spectra (2DCOS) derived from near-infrared (NIR) data as input, incorporating multi-scale convolution, dilated receptive fields, and squeeze-and-excitation (SE) attention mechanisms to extract spectral features [6-9]. A mixed-precision training strategy was further employed to improve training speed and computational efficiency [10]. A dataset was constructed using Poria cocos samples adulterated with lime powder, cassava starch, wheat flour, corn flour, and Pueraria powder across 21 gradient levels (0–100% at 5% intervals). Spectral features of the samples were obtained via NIR spectroscopy and 2DCOS, then input into the CNN model for regression analysis. Experimental results indicate that the proposed model significantly outperforms the traditional partial least squares (PLS) regression method in prediction accuracy and demonstrate strong generalization to complex adulteration scenarios. The study presents a novel, effective and accurate method for rapid adulteration detection in Poria cocos. It offers valuable support for quality control in traditional Chinese medicine, and has a wide range of applications.

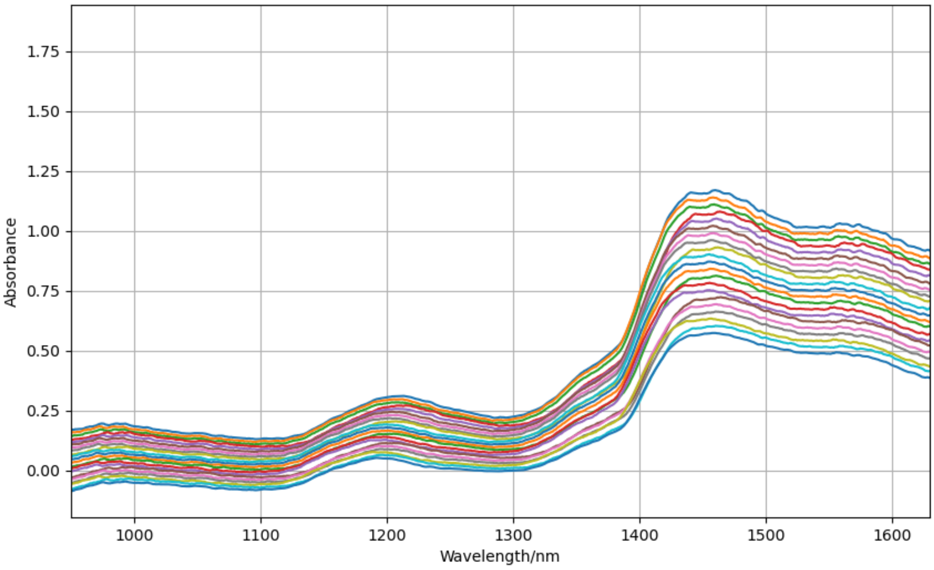
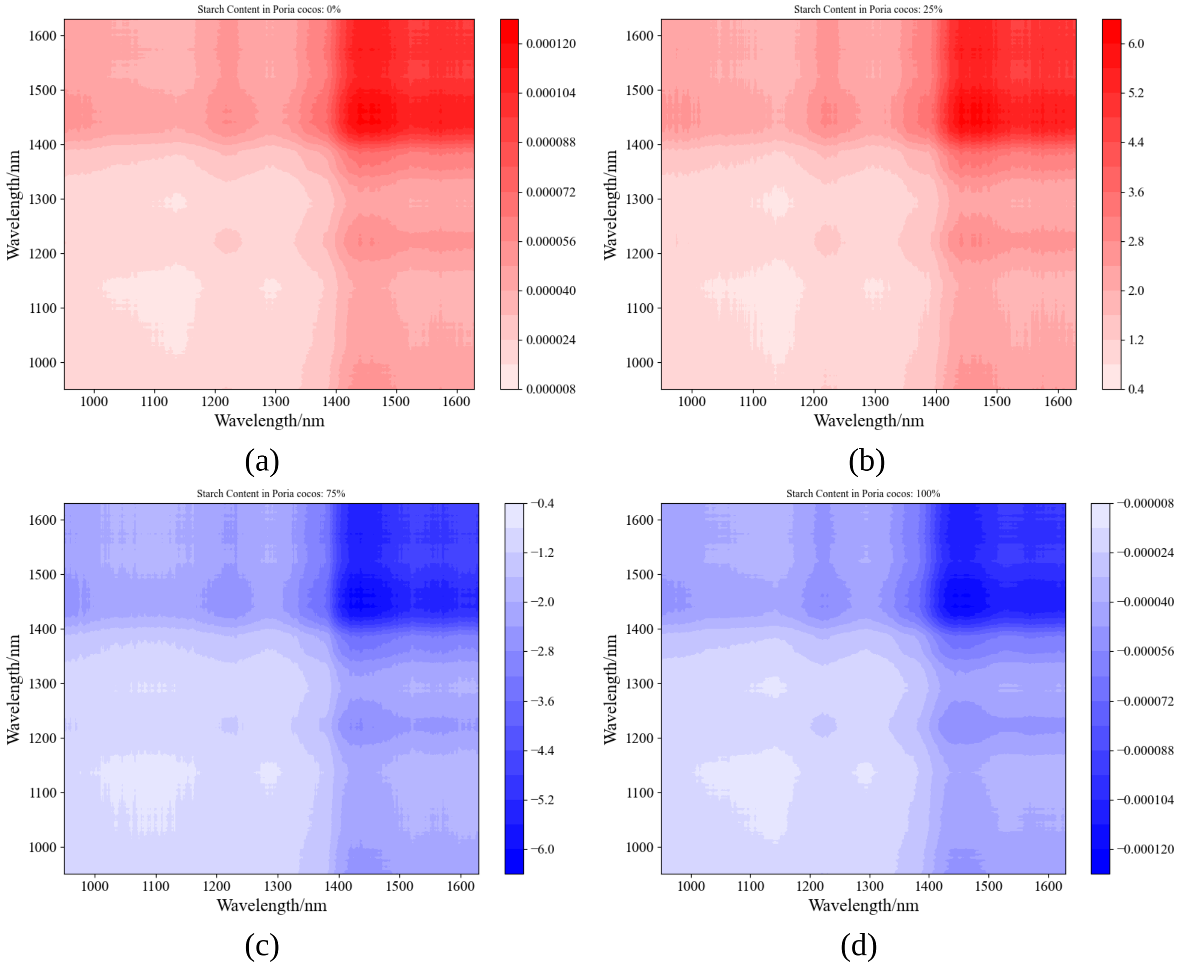


Figure 1 Near-infrared spectra of Poria cocos adulterated with different proportions of starches



(a) (b)

(c) (d)

Figure 2 The two-dimensional correlation spectra of Poria cocos adulterated with different proportions of starches (a) Starch Content in Poria cocos: 0% (b) Starch Content in Poria cocos: 25% (c) Starch Content in Poria cocos: 75% (d) Starch Content in Poria cocos: 100%

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Poster (P5)

2T2D STUDY OF LYMPHOCYTES IN INFECTIOUS MONONUCLEOSIS

N. Stach[1]*, A. Kurek*[1]*, M. Pietruszewska*[1]*, G. Biesiada*[2,3]*, J. Czepiel*[2,3]*, M. Birczyńska-Zych*[2,3]*,*
P. Moskal[1]*, M. Bociąga-Jasik*[2,3]*, and A. Wesełucha-Birczyńska*[1]
[1] *Faculty of Chemistry, Jagiellonian University, Kraków, Poland (e-mail: birczyns@chemia.uj.edu.pl) 2 Department of Infectious Diseases and Tropical Medicine, Medical College, Jagiellonian University, Kraków, Poland 3Department of Infectious Diseases, The University Hospital in Kraków, Kraków, Poland*

Raman spectroscopy has been extensively demonstrated as a powerful tool for the analysis of macromolecules characteristic of living organisms [1]. This research focuses on a detailed spectroscopic analysis of lymphocytes affected by infectious mononucleosis caused by Epstein-Barr virus (EBV, HHV-4) [2,3]. As it is proven, at least 98% of the population is infected with EBV, which makes it one of the most common viruses [4]. The primary aim of this study was to assess the capability of Raman spectroscopy to distinguish healthy lymphocytes from EBV-infected ones.

Blood samples were collected form patients suffering from infectious mononucleosis and receiving treatment at the University Hospital in Krakow. For comparative purposes, samples from healthy volunteers were also included. To guarantee detailed analysis, Raman spectra were acquired using two excitation wavelengths: 514.5 nm and 785 nm. 2D correlation method was performed with the Noda method [5,6]. Initially, mean Raman spectra presenting data for healthy and infected cells were calculated and subsequently used to generate synchronous and asynchronous 2D correlation maps.

Analysis of the asynchronous correlation spectra revealed distinct differences between healthy and diseased lymphocytes for both excitation wavelengths. For example, asynchronous peaks under 514.5 nm excitation indicate phosphorylation of Tyrosine, corresponding to activation of lymphocytes [2]. The detection of specific biochemical alternations shows potential of Raman spectroscopy as a non-invasive diagnostic tool in virial infections.

Acknowledgment
The study was supported by the research part of the subsidy of the Faculty of Chemistry Jagiellonian University in Krakow, Poland.
The study was carried out using research infrastructure funded by the European Union in the framework of the Smart Growth Operational Programme, Measure 4.2; Grant No. POIR.04.02.00-00-D001/20, "ATOMIN 2.0 – Center for materials research on ATOMic scale for the INnovative economy".

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Poster (P6)

A Cross-Spectral 2D-COS and Multimodal Deep Learning Framework for Wood Species Identification

Jing Liang, Xiaoxuan Xu, Jing Xu, Bin Wang*
College of Artificial Intelligence, Nankai University, Tianjin, 300350, China

Accurate identification of wood species is crucial in forest resource management and anti-smuggling efforts to prevent illegal logging and protect ecological sustainability. Traditional morphology-based methods are time-consuming, labor-intensive, and require specialized expertise. In recent years, deep learning has emerged as a promising approach for wood species classification due to its ability to automatically extract discriminative features [1]. However, relying on a single spectral modality often fails to capture the complex structural composition of wood.

Near-infrared (NIR) spectroscopy is sensitive to overtones and combination bands of organic functional groups, while mid-infrared (MIR) spectroscopy directly probes molecular vibrations and crystalline structures. Their integration provides complementary chemical information. In this study, 27 wood species were systematically measured using both NIR and MIR spectroscopy. A novel classification framework based on cross-spectral two-dimensional correlation spectroscopy (2D-COS) and a multimodal deep learning network is proposed[2].

The multimodal fusion network significantly outperforms unimodal models due to the complementary nature of NIR and MIR data. The introduction of weighted 2D-COS further enhances feature extraction by emphasizing key spectral regions, leading to improved classification accuracy compared to unweighted approaches. Interpretability analysis reveals distinct fingerprint regions in both MIR and NIR spectra, such as lignin-associated peaks recognized as important features by the model.

Moreover, physics-informed 2D-COS augmentation and decoupled representation learning strategies effectively address the long-tailed distribution problem often encountered in wood spectral datasets. Compared with traditional single-spectrum approaches, the proposed cross-spectral 2D-COS method incorporates prior physical knowledge and leverages a multi-channel network architecture to integrate NIR and MIR information more effectively. This framework offers promising potential for applications in forestry monitoring and illegal timber trade detection, and advances the intersection of spectroscopy and deep learning in material identification.

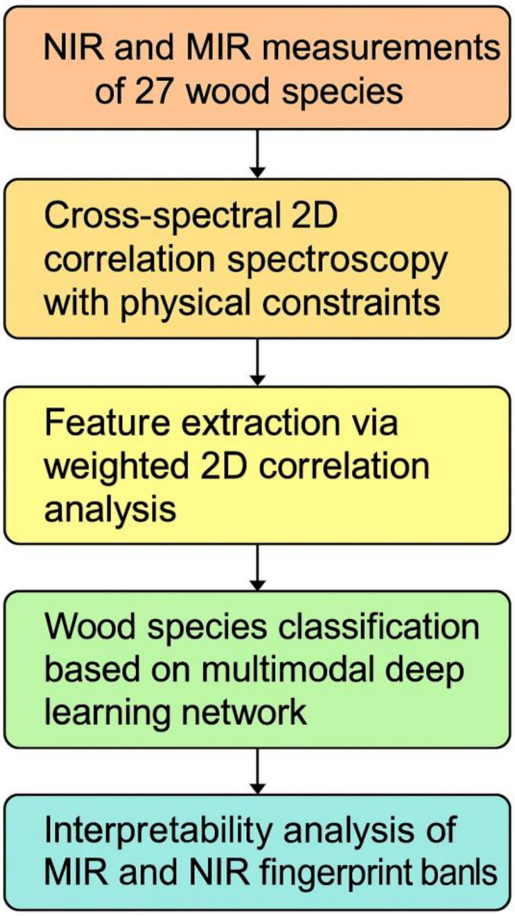

Figure 1 Workflow diagram

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Poster (P7)

A Multi-Task Detection Approach for Meat Adulteration Based on Two-Dimensional Correlation Spectroscopy and Deep Learning

Jing Liang, Xiaoxuan Xu, Jing Xu, Bin Wang*

College of Artificial Intelligence, Nankai University, Tianjin, 300350, China

With the growing demand for meat products, adulteration in meat has become increasingly common. Thickening agents such as carrageenan are frequently added to pork, beef, and chicken to enhance weight and texture [1]. Although conventional analytical methods—such as high-performance liquid chromatography (HPLC), polymerase chain reaction (PCR), and mass spectrometry (MS)—offer high accuracy, they are typically costly and time-consuming. In contrast, near-infrared (NIR) spectroscopy is a rapid, non-destructive, and reagent-free technique that has been widely employed in food safety monitoring[2]. Two-dimensional correlation spectroscopy (2D-COS) further enhances spectral resolution by expanding overlapped peaks in one-dimensional spectra into a two-dimensional domain via synchronous and asynchronous correlation analysis under controlled perturbations[3].

Leveraging the powerful nonlinear fitting capabilities of deep learning, this study explores the detection of meat adulteration by integrating 2D-COS with advanced neural network architectures. We developed an end-to-end deep learning framework that simultaneously performs meat species classification and carrageenan concentration regression using dual-instrument near-infrared (NIR) spectral data. By incorporating dynamic two-dimensional correlation spectroscopy (2D-COS) for feature enhancement and an instrument-adaptive attention mechanism, the framework effectively addresses challenges posed by inter-instrument variability and limited sample size. Experimental results demonstrate that the proposed method offers notable advantages in terms of cross-instrument generalization and low-concentration detection sensitivity.

This method enables feature extraction grounded in physical and chemical interpretation, and interpretability analyses further validate the relevance of critical spectral regions, enhancing the model's reliability. Comparative experiments demonstrate the superiority of deep learning over traditional approaches, highlighting its potential as an efficient and robust solution for food adulteration detection. Furthermore, the proposed cross-instrument data fusion strategy offers a practical reference for integrating heterogeneous spectral data, presenting valuable implications for real-world deployment in food safety applications.

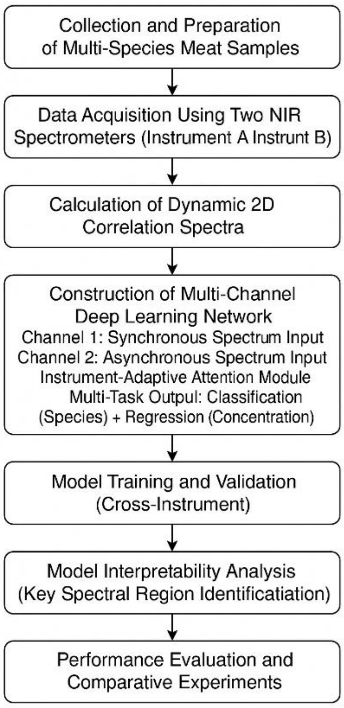

Figure 1 Workflow diagram

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Poster (P8)

Qualitative and Quantitative Analysis of High-Quality Adulterated Meat Based on a Synchronous-Asynchronous Spectra Co-Characteristic Learning Network

*Mingyue Huang, Zhenbing Lu, Yongtao Liu, Bin Wang**
College of Artificial Intelligence, Nankai University, Tianjin, 300350, China

To address the issue of characteristic confusion and reduced model prediction accuracy caused by the direct superposition of two-dimensional (2D) correlation synchronous and asynchronous spectra, this study proposes a two-dimensional deep learning model based on 2T2D correlation spectroscopy for co-characteristic extraction from synchronous and asynchronous spectra[1-5]. The model is applied for qualitative and quantitative prediction of adulterated beef with duck meat and adulterated mutton with chicken meat. The proportion of duck meat in adulterated beef and chicken meat in adulterated mutton ranges from 0.5% to 95%. Figure 1 shows the one-dimensional (1D) spectral of adulterated beef and mutton with varying levels of adulteration. 2D correlation analysis was performed on the spectra of the two types of adulterated meat using content as the perturbation. Figure 2 presents the synchronous and asynchronous content-peturbed 2D correlation spectra of beef and mutton. Based on these 2D correlation spectra and a co-characteristic learning network, qualitative and quantitative prediction models were established for detecting duck meat in beef and chicken meat in mutton. This method takes the synchronous and asynchronous 2D correlation spectra as input and employs independent characteristic extraction modules for each, enabling efficient and comprehensive extraction of their respective spectra characteristic. Subsequently, a channel attention mechanism is applied to the extracted characteristic for weighted fusion, enhancing the representation of key information. The fused characteristic are then further processed and used for classification and regression outputs. To increase the network depth for effective learning of complex 2D spectral characteristic while avoiding gradient vanishing or explosion issues, residual modules are incorporated into the model. In addition, Inception modules are integrated to extract multi-scale feature information, thereby enhancing the model's representation capability. This approach enables the extraction of characteristic from different dimensions of the synchronous and asynchronous spectra independently, thereby avoiding mutual interference. The channel attention mechanism allows the model to adaptively select important characteristic information, improving both prediction accuracy and precision.

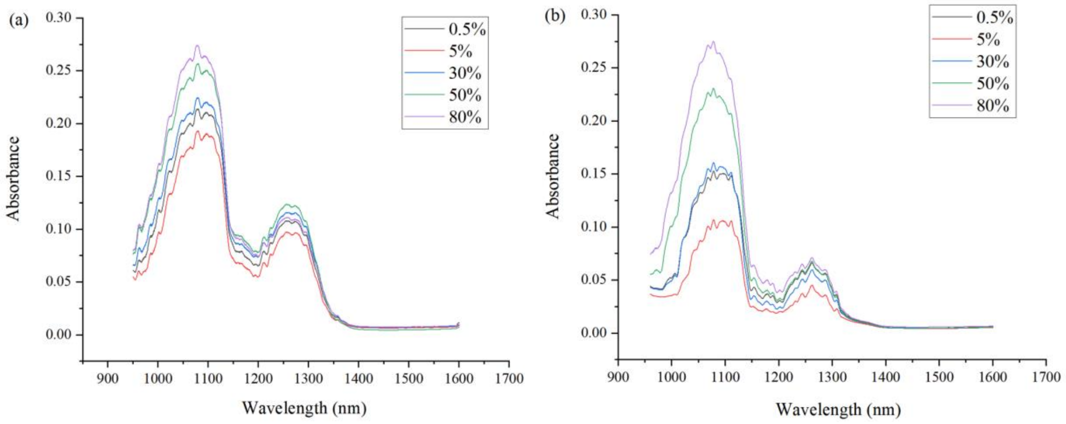

Figure 1. One-dimensional spectral profiles, (a) Beef adulterated with varying levels of duck meat, (b) Mutton adulterated with varying levels of chicken meat

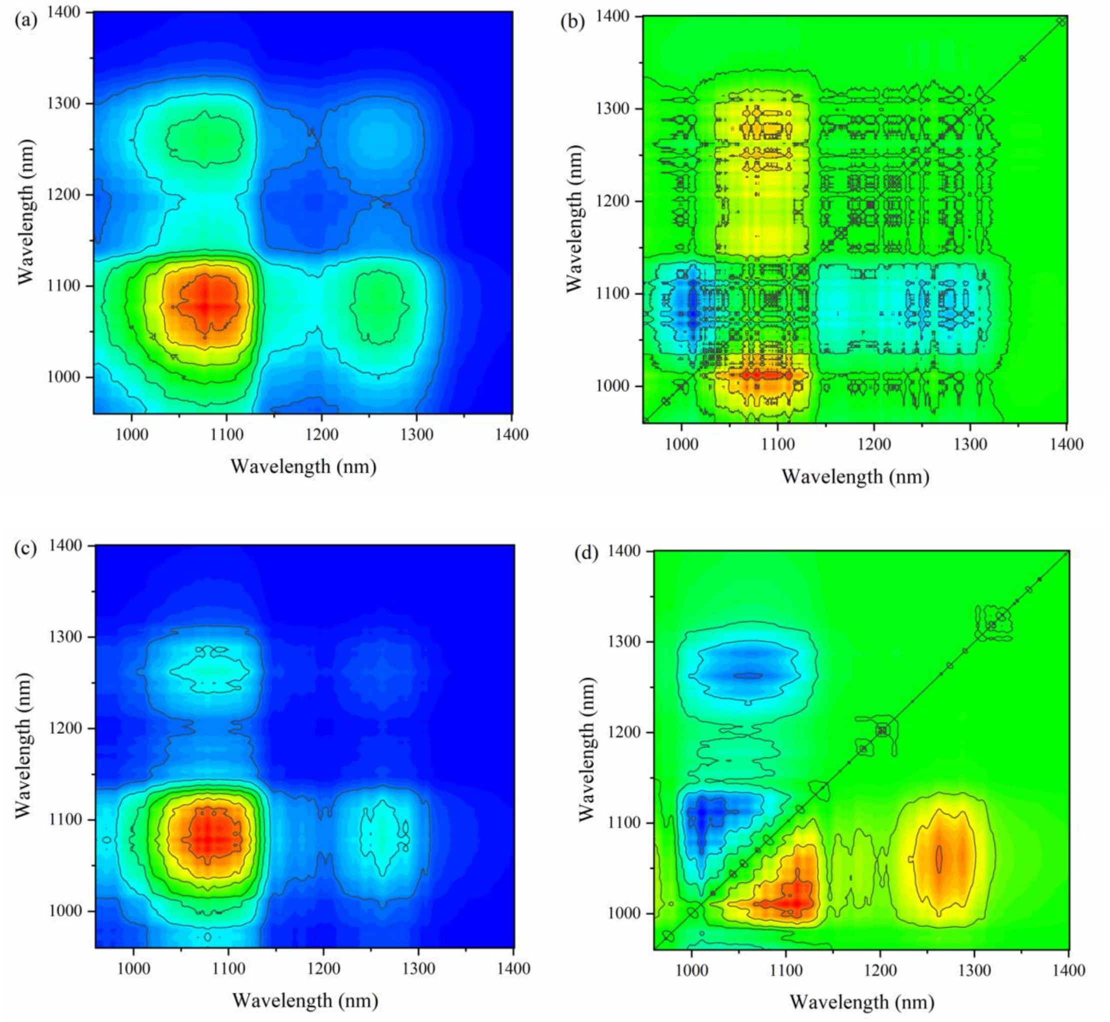

Figure 1. 2D correlation spectra, (a) Synchronous spectrum of beef adulterated with 50% duck meat, (b) Asynchronous spectrum of beef adulterated with 50% duck meat, (c) Synchronous spectrum of mutton adulterated with 50% chicken meat, (d) Asynchronous spectrum of mutton adulterated with 50% chicken meat.

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Poster (P9)

COMPONENT IDENTIFICATION OF THE OCHRE AND PROCESSING OCHRE USING 2T2D CORRELATION RAMAN SPECTROSCOPY

Bo Yang[a], *Shu-Min Wang*[a], *Young Mee Jung*[b],
[a] *School of Pharmaceutical Sciences, Changchun University of Chinese Medicine, Changchun 130117, PR China*
[b] *Department of Chemistry, Institute for Molecular Science and Fusion Technology, Kangwon National University, Chuncheon 24341, Republic of Korea*

Ochre is a widely used mineral medicines in clinical practice, particularly in China and several other countries, valued for its distinctive therapeutic effects and broad applications. However, due to the lack of standardized processing methods and quality control standards, inconsistencies in its market quality of the ochre medicinal materials persist. In addition, the mechanism underlying ochre's pharmacological effects and traditional processing techniques remain poorly understood, which seriously affect the quality and clinical efficacy of ochre medicines. In this study, we employed two-trace two-dimensional (2T2D) correlation Raman spectroscopy to identify the mineral medicines and to elucidate their processing mechanisms from a chemical perspective[1]. 2T2D correlation Raman spectroscopy allowed us to detect the compositional changes in the ochre samples following calcination and vinegar quenching, revealing molecular-level alterations that clarify the processing mechanism of ochre. This is the use of 2T2D correlation analysis to explore the processing mechanism for traditional Chinese medicine (TCM). Our findings provide new approaches and references for the quality detection and safe clinical application of TCM[2]. Most importantly, the novel application of 2T2D correlation Raman spectroscopy provides new insights into the study of TCM and reveals the processing mechanism of mineral medicines.

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Poster (P10)

INVESTIGATION ON THE INTERACTION BETWEEN TECTORIDIN AND AMYLOPECTIN SUBSTANCES USING THE DAOSD APPROACH

Ying Zhang[1], Ming Ren[3], Gui-xin Zou[1], Yi-zhuang Xu[2*]
1The Second Affiliated Hospital of Liaoning University of Traditional Chinese Medicine, Shenyang, Liaoning 110034, China
2Beijing National Laboratory for Molecular Sciences, State Key Laboratory for Rare Earth Materials Chemistry and Applications, College of Chemistry and Molecular Engineering, Peking University, Beijing, 100871, PR China
3College of Pharmacy, Liaoning University of Traditional Chinese Medicine, Dalian, Liaoning Province, 116600, PR China
* Corresponding author: Yi-Zhuang Xu (xyz@pku.edu.cn)

Tectoridin, an isoflavonoid compound and an active component of the traditional Chinese medicine *Belamcanda chinensis* （L.）DC., was extracted and identified from the plant *Iris tectorum* Maxim by Shibata, a Japanese scholar, in 1928.Tectoridin and its intestinal bacterial hydrolyzate, tectorigenin, exhibit a broad spectrum of biological activities, demonstrating potential therapeutic effects on inflammatory disorders such as pneumonia[1], anti-rheumatoid arthritis[2], severe acute pancreatitis[3], and osteoarthritis[4].

Rice-washed water is a commonly used excipient in the processing of Chinese medicinal materials. It is an aqueous solution of glutinous rice flour, mainly containing amylopectin, which is used to remove excess oil in traditional Chinese medicine and reduce the pungent odor and slippery bowel effect of the drug. *Belamcanda chinensis*（L.）DC. commonly used Rice-washed water for processing.

As elucidated in scientific literature, the interaction between polyphenols (including flavonoids) and starch can be attributed to dual molecular mechanisms: firstly, the hydrophobic domains of flavonoids facilitate the formation of V-type inclusion complexes by interacting with the hydrophobic cavities within starch helical structures through non-covalent hydrophobic interactions[5,6]; secondly, the polyhydroxylated and carbonyl-containing scaffolds of these compounds enable additional stabilization via hydrogen bonding and van der Waals forces with starch polymers, collectively promoting molecular aggregation phenomena[7].

Figure 1 shows the structure of tectoridin. With multiple hydroxyl polar groups, tectoridin molecules form hydrogen bonds, leading to poor hydrophilicity and low water solubility, which restricts its application. In this study, an asynchronous orthogonal sample design was used. Tectoridin concentration was set as a perturbation to create a 2D asynchronous spectrum of an tectoridin-amylopectin mixed solution. By analyzing the cross-peaks of the asynchronous spectrum, we studied the peak width and position changes of tectoridin, explored the interaction between amylopectin and tectoridin, and investigated the solubility enhancement mechanism from a molecular perspective.

2. Experimental

2.1. Reagents

Tectoridin with purity of 98.7% was purchased from National Institutes for Food and Drug Control. Amylopectin was purchased from Aladdin. Methanol (HPLC grade) was acquired from Fisher Scientific.

2.2 Instrumentation

The UV-Vis spectra were acquired using a Shimadzu UV-2600i spectrophotometer (Shimadzu Corporation, Kyoto, Japan), with all measurements performed in absorption mode at a medium scan rate.

2.3 Spectroscopic experiments

A series of 70% methanol solutions with different concentrations of tectoridin were prepared, and their UV-VIS spectra were recorded. Subsequently, the absorbance at 265 nm from each UV-VIS spectrum was plotted against the concentration of tectoridin. A good linear relationship was obtained (R^2=0.9984) (**Figure 2**). Based on these results, the appropriate concentration range for tectoridin was selected as 1.83–5.49 ng/L, and the concentration series was designed accordingly.

Multiple series of 70% methanol solutions containing tectoridin and amylopectin were prepared. The UV-VIS spectra of these solutions were collected and used. Each set of UV-VIS spectra was used to construct 2D asynchronous spectra through a program written by our laboratory using MATLAB software.

3. Results and Discussion

The one-dimensional spectra of the tectoridin-amylopectin mixed solutions used to construct the two-dimensional asynchronous spectrum are shown in Fig. 3(A). The two-dimensional asynchronous spectrum constructed by Matlab program according to the calculation method is presented in Fig.3 (B). In the two-dimensional correlation spectrum, red represents that the cross peak is a positive peak, and blue represents that the cross peak is a negative peak.The Double Asynchronous Orthogonal Sample Design Scheme (DAOSD) was implemented to establish concentration gradients for preparing a series of solutions containing tectoridin and amylopectin. Analysis of the two-dimensional asynchronous spectrum revealed two cross-peak pairs, whose presence unambiguously indicates intermolecular interactions between these compounds. The spectral patterns of these cross-peaks provide critical information regarding conformational changes subsequent to molecular recognition events.

The cross peak at (240 nm, 270 nm) in the 2D asynchronous spectrum is a negative peak, stronger than the negative peak at (300 nm, 270 nm). The cross peak at (270 nm, 240 nm) is a positive peak, more intense than the positive peak at (270 nm, 300 nm). This 2D asynchronous spectrum shows increased peak position and reduced peak width. It is speculated that as the supramolecular polymer of tectoridin and amylopectin forms, the maximum absorption peak shifts to a longer wavelength (red shift), indicating reduced environmental polarity around tectoridin due to amylopectin addition. This suggests that the polar solvent around tectoridin in the inclusion complex is replaced by hydrophobic groups within amylopectin. Tectoridin and amylopectin exhibit strong van der Waals and hydrophobic interactions, forming an inclusion complex. The decreased peak width implies restricted molecular motion in the system, indicating that tectoridin interacts with the hydrophobic region in the starch cavity and can form an inclusion complex with amylopectin. In summary, amylopectin can interact with tectoridin to enhance its solubility.

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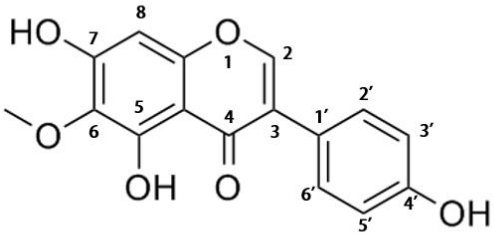


Figure 1 Molecular structure of tectoridin

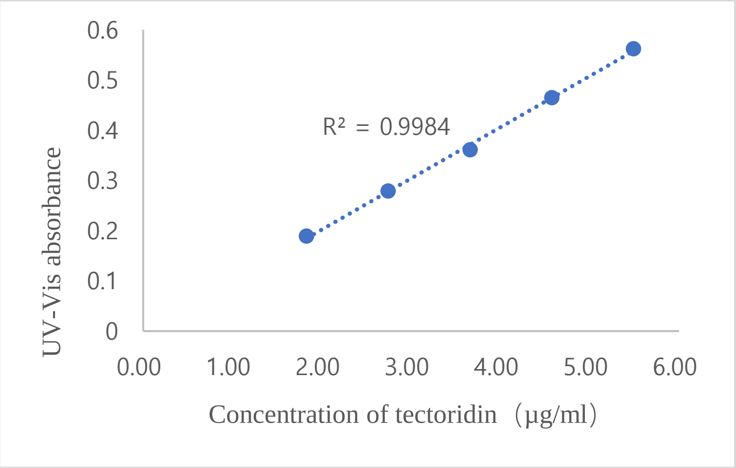
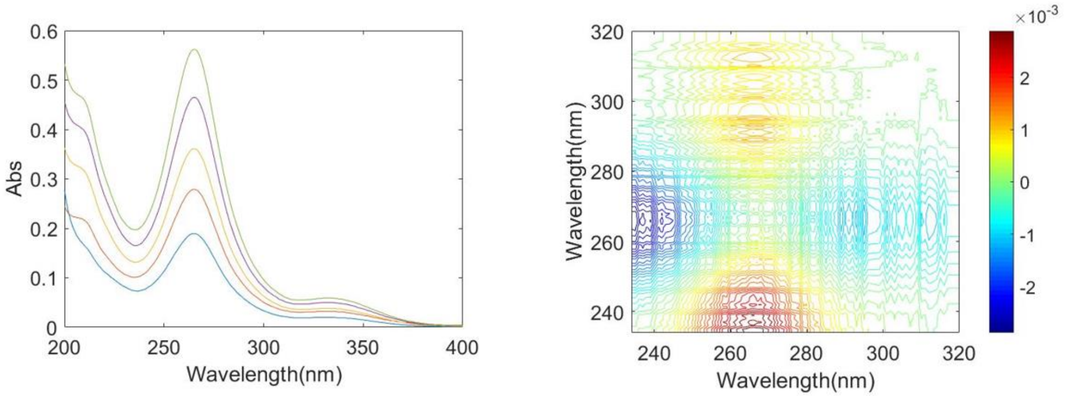


Figure 2 Linear relationship between the absorbance at 265 nm in UV-Vis spectra of aqueous solution and tectoridin and concentration of tectoridin



A

B

Figure 3 1D spectrum (A) and 2D asynchronous spectrum (B) of the tectoridin-amylopectin system.

Poster (P11)

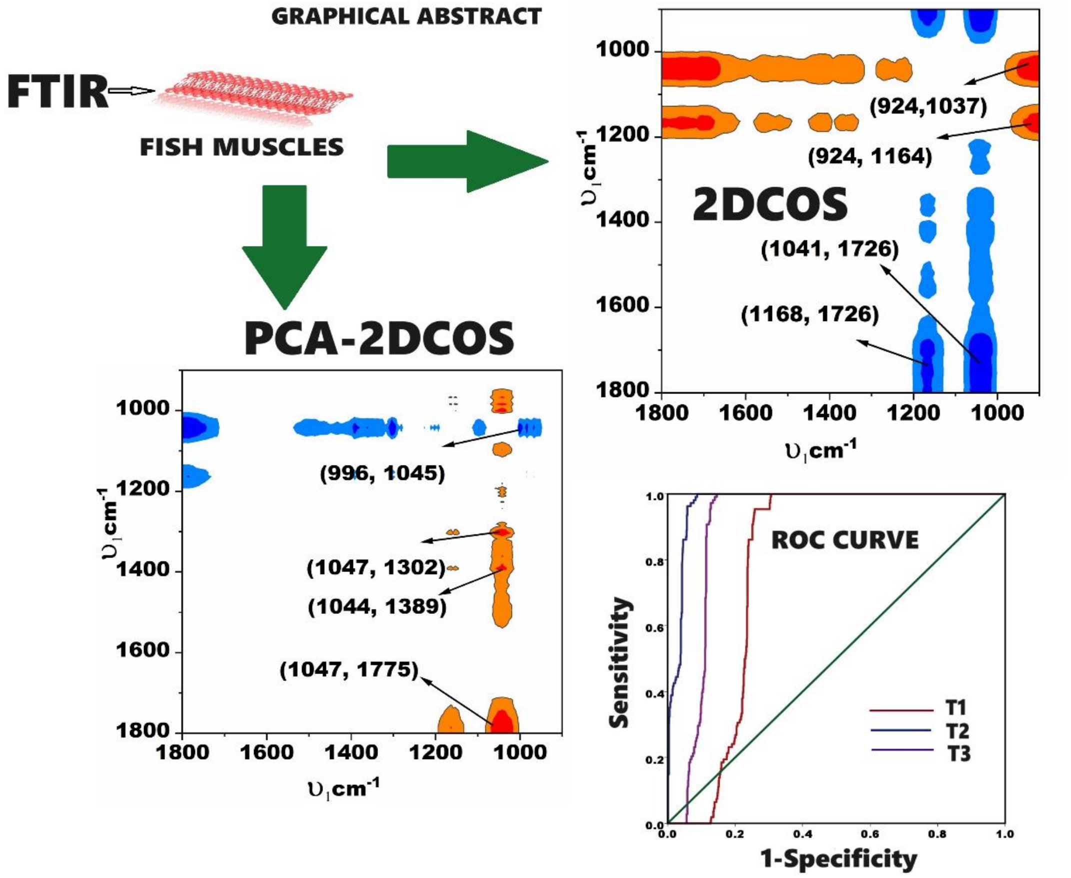
DISSECTING SUBTLE BIOMOLECULAR PERTURBATIONS IN FISH MUSCLE UNDER ZN STRESS USING PCA-COUPLED 2D-COS-FTIR AND ROC ANALYSIS

S. Karthikeyan

Department of Physics, Dr. Ambedkar Government Arts College, Chennai 600039, Tamil Nadu, India. physicskarthik@gmail.com, physicskarthik@dagac.edu.in

Two-dimensional correlation spectroscopy (2DCOS) applied to FTIR enhances spectral resolution, enabling detailed analysis of complex biological samples. In biomolecular studies, it allows for the clear identification of proteins, lipids, and carbohydrates by resolving overlapping bands. Synchronous spectra highlight simultaneous molecular changes, with key signals observed in the amide bands (proteins), (lipids), and carbohydrate-associated vibrations. The main goal of this research is to examine the impact of zinc toxicity on fish exposed under controlled conditions, utilizing two-dimensional correlation spectral analysis. This method offers greater sensitivity compared to conventional one-dimensional spectra, as it can detect subtle spectral variations caused by external stressors that might otherwise go unnoticed. Synchronous correlation maps revealed major spectral changes, particularly in proteins (1668 cm^{-1}), phospholipids (1771 cm^{-1}), and fatty acids (1707 cm^{-1}). The asynchronous spectra indicated that alterations began with the phosphodiester stretching in glycogen, followed by changes in the Amide I band. Additionally, the integration of principal component analysis (PCA) with two-dimensional spectral analysis highlighted weak yet detectable shifts in the Amide III region associated with proteins.Furthermore, hetero-asynchronous correlation spectra displayed distinct cross peaks at +(1047, 1389), enhancing spectral resolution. This investigation provides valuable insight into the biochemical changes in the muscle tissues of *Gambusia affinis* subjected to zinc toxicity, using advanced two-dimensional correlation infrared spectroscopy.PCA-coupled 2DCOS analysis significantly enhanced spectral resolution compared to conventional 2DCOS, revealing subtle biomolecular changes in fish under Zn exposure. Notably, well-resolved Amide III peaks at 1335 cm^{-1} were detected, which were previously masked by lipid peaks at 1364 cm^{-1}. PCA-based analysis also clarified glycogen-related changes in carbohydrate metabolism and uncovered protein structural transitions from α-helix to β-sheet and β-turn. Additionally, lipid-associated peaks at 2952 cm^{-1}, obscured in standard spectra, were distinctly identified. ROC analysis confirmed the reliability and sensitivity of PCA-2DCOS in detecting Zn-induced biochemical alterations.

Key words 2DCOS, FTIR, Proteins, lipids, PCA-2DCOS



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Poster (P12)

ANALYSIS OF CRYSTALLINITY CHANGES IN BIODEGRADABLE POLYMER-BASED SOLID POLYMER ELECTROLYTES USING 2D CORRELATION SPECTROSCOPY

Sujin Lee[a], Yeonju Park[a,b], Siwoo Kim[a], Isao Noda[c,d], Young Mee Jung[a,b,*]

[a]*Department of Chemistry, Institute for Molecular Science and Fusion Technology, Kangwon National University, Chuncheon 24341, Korea*
[b]*Kangwon Radiation Convergence Research Support Center, Kangwon National University, Chuncheon 24341, Korea*
[c]*Department of Materials Science and Engineering, University of Delaware, Newark, DE 19716, USA*
[d]*Danimer Scientific, 140 Industrial Blvd., Bainbridge, GA 39817, USA*
ymjung@kangwon.ac.kr

Solid polymer electrolytes (SPEs) have recently emerged as a promising material for next-generation Li-ion batteries (LIBs). As electrolyte that derivers ions through polymer chains, SPEs can enhance safety by eliminating the flammability risks associated with organic solvents in liquid electrolytes. In addition to improved safety, SPEs offer higher energy density than conventional LIBs and provide advantages such as excellent interface compatibility, simple processing, and cost-effectiveness. However, their ionic conductivity remains lower than that of other solid electrolytes. A key factor affecting this conductivity is the crystallinity of the polymer-higher crystallinity generally hinders ion transport efficiency.[1]

To investigate the relationship between crystallinity and ionic conductivity, the electrochemical impedance and temperature-dependent IR spectra of poly(hydroxybutyrate-*co*-hydroxyhexanoate) (PHBHx)-polyvinyl acetate (PVAc) blends were measured. At room temperature, the IR spectra of PHBHx/PVAc blends with a higher PVAc content resemble those of pure PHBHx observed above its melting temperature (*Tm*), suggesting that increased PVAc content acts as a solvent to reduce PHBHx crystallinity. The detailed findings will be discussed in the presentation.

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Poster (P13)

ADSORPTION CHARACTERISTICS AND ADSORPTION MECHANISM OF CHLOROPHENANTHRENE ON POLYSTYRENE WITH DIFFERENT PARTICLE SIZES

*Gui-Mei Dong, Ji-Yuan He, Shu-jie Zhang, Ren-Jie Yang**
College of Engineering and Technology, Tianjin Agricultural University, Tianjin, 300384
**rjyang1978@163.com*

In order to elucidate the mechanism of particle size on the adsorption of organic pollutants by microplastics, the present study was carried out to investigate the adsorption characteristics and mechanism of chlorophenanthrene adsorption by typical microplastic polystyrene (PS, 30 mesh/60 mesh/100 mesh) through adsorption kinetics, isotherm experiments combined with the technique of two-dimensional infrared correlation spectroscopy. The results showed that the adsorption capacity and rate of small-size PS100 were significantly better than that of large-size PS due to the larger specific surface area (0.580-0.672 m^2/g), more developed pore structure (pore volume 0.133 mL/g) and more abundant surface active sites. The adsorption behaviors were consistent with pseudo-secondary kinetics ($R^2 \geq 0.99$) and Freundlich model ($R^2=0.78$-0.92), confirming that the adsorption mechanism was shifted from physical partitioning to surface chemical adsorption due to the decrease in particle size; the infrared spectroscopy and the 2D correlation analysis further revealed that the adsorption was mainly dependent on hydrophobic interaction and π-π stacking, and the molecular movement of PS was more active in small particle sizes, and the surface effect strengthened the pollutant interaction. This study reveals that the particle size dominates the adsorption mechanism by regulating the surface properties, which highlights the high risk of small-sized microplastics in environmental composite pollution and provides a theoretical basis for the assessment of the environmental behavior of microplastics and pollutants.

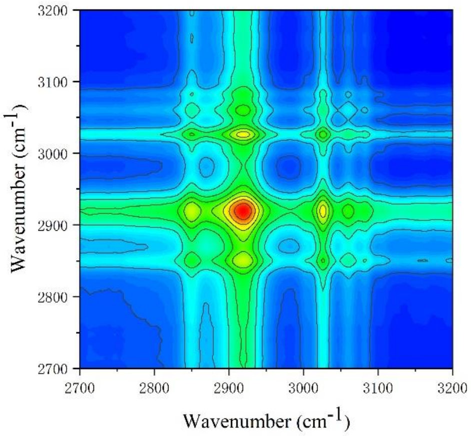

Fig.1 2D synchronous spectra of adsorbed PS60

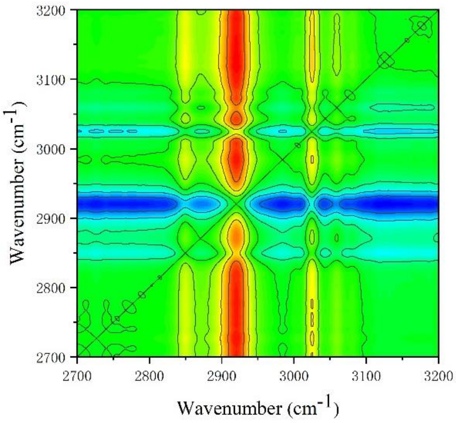

Fig.2 2D asynchronous correlation spectra of adsorbed PS60

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Poster (P14)

FORMATION OF HYDRATED HYDROGEN IONS DURING THERMAL DECOMPOSITION OF SCANDIUM CHLORIDE

Anqi He, Ran Guo, Yizhuang Xu

College of Chemical and Molecular Engineering, Peking University, Beijing, 100871, China

The formation of hydrated hydrogen ions in gaseous systems remains a fundamental question in chemistry. While H_3O^+ is commonly represented in textbooks for aqueous solutions, the actual existence of these species in gas-phase conditions requires investigation. This study employed thermogravimetric analysis coupled with infrared spectroscopy and mass spectrometry (TGA-FTIR-MS) to investigate the thermal decomposition of crystalline scandium chloride hexahydrate ($ScCl_3{\cdot}6H_2O$).

The sample was heated at 20°C/min to 300°C under nitrogen atmosphere. Evolved gases were analyzed using three-dimensional asynchronous correlation spectroscopy, enabling separation of overlapping spectral contributions from different gaseous components. This method identifies pure component spectra even when conventional analysis fails due to severe peak overlap.

Initial infrared analysis revealed gaseous water (H_2O) and hydrogen chloride (HCl) in the decomposition products. However, three-dimensional correlation spectroscopy indicated additional spectral signals beyond these components, suggesting a third chemical species in the gaseous effluent.

Mass spectrometric analysis provided crucial evidence for ion formation. A significant peak at m/z=37 was attributed to the Zundel cation ($H_5O_2^+$), with an intensity ratio to combined HCl peaks of approximately 5.2×10^{-2}. This indicates that while ionization occurs, hydrated ion concentration remains less than one-tenth that of molecular HCl.

Statistical analysis confirmed H_3O^+ ions (m/z=19) above background noise. The temporal evolution curves of m/z=19 and m/z=18 signals showed distinct shapes (correlation coefficient 0.72), and the intensity ratio (0.099%) significantly exceeded natural deuterium abundance (0.015%), ruling out HOD^+ as the sole contributor.

The results demonstrate that gaseous HCl can undergo ionization when coexisting with water vapor, forming primarily $H_5O_2^+$ and smaller amounts of H_3O^+. No evidence was found for $H_7O_3^+$ (Eigen cation) or more complex hydrated species, likely due to lower thermal stability at experimental temperatures.

Compared to weak acids like acetic acid, which showed no detectable gas-phase ionization, HCl exhibits greater propensity for H-Cl bond dissociation and subsequent reaction with water molecules. The preferential formation of $H_5O_2^+$ over H_3O^+ suggests that cooperative interaction of two water molecules with a proton provides enhanced stabilization.

Gas-phase ionization extent is dramatically reduced compared to aqueous solutions, where HCl undergoes complete dissociation. This difference reflects the absence of high dielectric constant medium that normally screens Coulombic attractions between ions in solution.

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Poster (P15)

INVESTIGATION OF THE INTERACTION BETWEEN ASTRAGALIN AND CALF THYMUS DNA USING TWO-DIMENSIONAL CORRELATION SPECTROSCOPY

Yi Wu, Da Li, Yizhuang Xu
College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, China

Astragalin[1], a flavonoid glycoside from herbs like Astragalus membranaceus and Eucommia ulmoides, exhibits significant anti-tumor, anti-depressant, and antioxidant activities. DNA[2] serves as a critical drug target, especially for anti-tumor agents. Small molecules like astragalin can interact with DNA via reversible non-covalent binding (electrostatic, groove binding, or intercalation), altering its structure/function to regulate cellular processes. These interactions hold high value for drug design.

This study innovatively employs two-dimensional correlation spectroscopy[3] (2DCOS) to dynamically probe the micro-mechanism of astragalin's interaction with calf thymus DNA (ctDNA). We systematically investigate their binding mode to comprehensively elucidate the molecular mechanism, providing critical support for understanding astragalin's pharmacology and developing DNA-targeted drugs.

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Poster (P16)

APPLICATION OF TWO-TRACE TWO-DIMENSIONAL CORRELATION SPECTROSCOPY FOR THE ANALYSIS OF AMANITA MUSCARIA SAMPLES RAMAN SPECTRA

T. Punko, A. Wesełucha-Birczyńska
Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, str., 30-387
Krakow, Poland
timofey.punko@student.uj.edu.pl

Hundreds of years ago, in primitive societies people used the fly agaric in shamanic practices and rituals. Thanks to its psychoactive properties, even now, many years later, people are interested in the influence of chemical compounds contained in mushrooms on the human body and its consciousness. Nowadays, the common belief about the toxicity of Amanita Muscaria is changing, and the mushroom has even been included in alternative medicine. Based on new experiences, scientific research appears to confirm the benefits and potential use of the mushroom as a source of pharmaceutical substances. This work describes not only the properties of Amanita Muscaria, but also its study using Raman spectroscopy and two-dimensional correlation spectroscopy application to analyze the spectra. The main active substances of Amanita Muscaria are muscarine and ibotenic acid – a mushroom toxin that is transformed into the psychoactive compound muscimol after heat treatment.[1] Raman spectroscopy as a non-destructive method, which does not require special preparation of the sample, allowed obtaining spectra, that enabled the analysis of the components of the mushroom.[2] Two-trace two-dimensional correlation spectroscopy allowed for a precise analysis of the common features and differences between the spectra of mushroom samples differing in the sample preparation method.[3]

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Poster (P17)

EFFICIENT CLASSIFICATION OF FUNGAL RAMAN SPECTRA VIA DUAL-CHANNEL ATTENTION CNN-LSTM BASED ON SYNCHRONOUS AND ASYNCHRONOUS 2D CORRELATION SPECTRA

Hailong Feng, *Bin Wang*

College of Artificial Intelligence, Nankai University, Tianjin, 300350, China

Raman spectroscopy, with its advantages of being non-destructive, rapid, and highly molecule-specific, plays a vital role in the identification of microbial species, especially fungi. However, conventional methods often struggle to extract high-level features from complex spectra, resulting in suboptimal classification accuracy. In this study, we propose an innovative deep learning framework that integrates synchronous and asynchronous two-dimensional correlation spectra with a dual-channel attention CNN-LSTM for accurate fungal Raman spectra classification. Specifically, Raman spectra from various fungal samples are collected and preprocessed, followed by the construction of synchronous and asynchronous 2D correlation spectra to capture both co-varying and asynchronous features among wavenumbers. A dual-channel convolutional neural network is then designed to separately extract spatial features from synchronous and asynchronous spectra. Attention mechanisms are incorporated to enhance the model's focus on key spectral regions, while LSTM layers are employed to mine sequential correlations within the spectral features. Finally, multi-channel feature fusion enables high-precision classification of fungal samples. Experimental results demonstrate that the proposed method achieves significantly higher classification accuracy and stronger generalization ability compared to conventional CNNs and single-channel approaches. This research provides a novel strategy for intelligent analysis and automatic recognition of complex microbial spectral data.

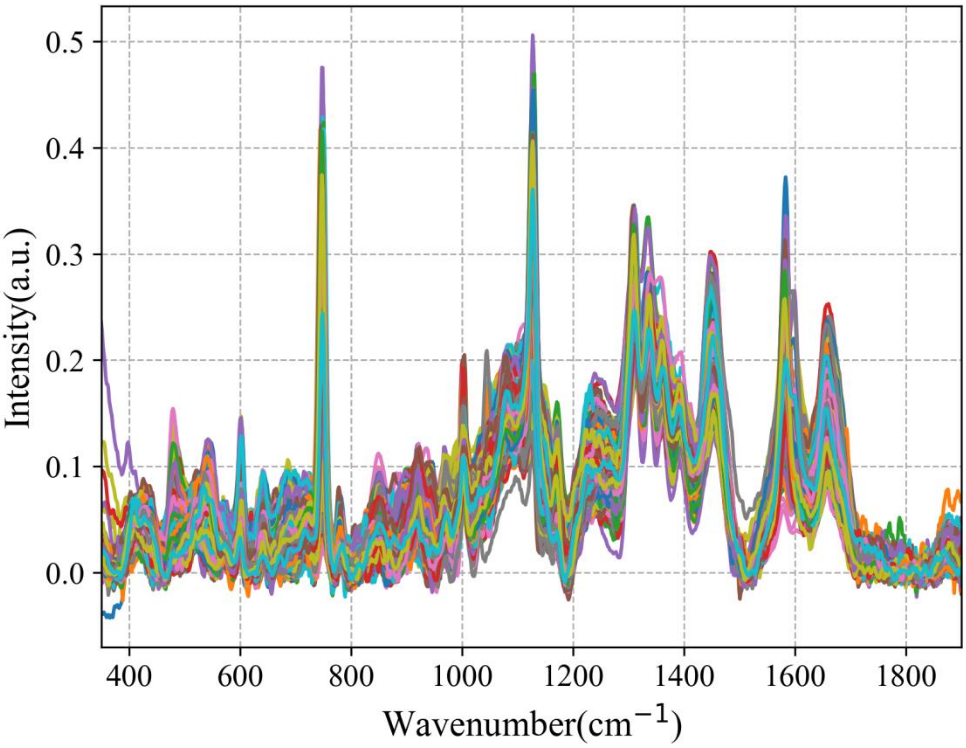

Figure 1. One-dimensional raman spectrum of fungi

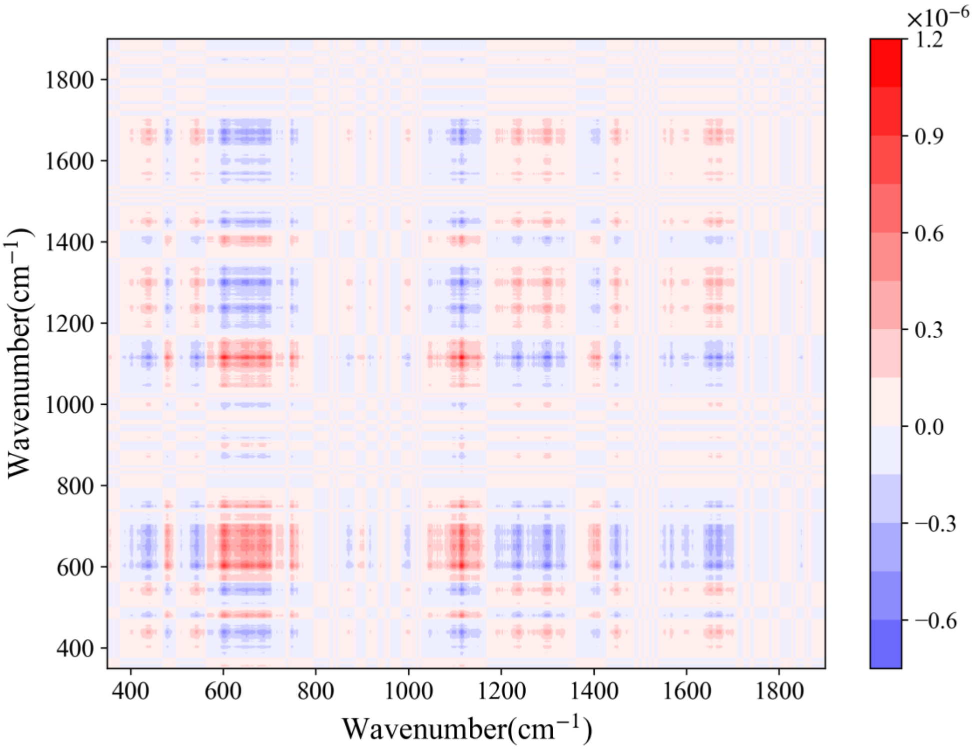

Figure 2. synchronous 2D correlation spectra

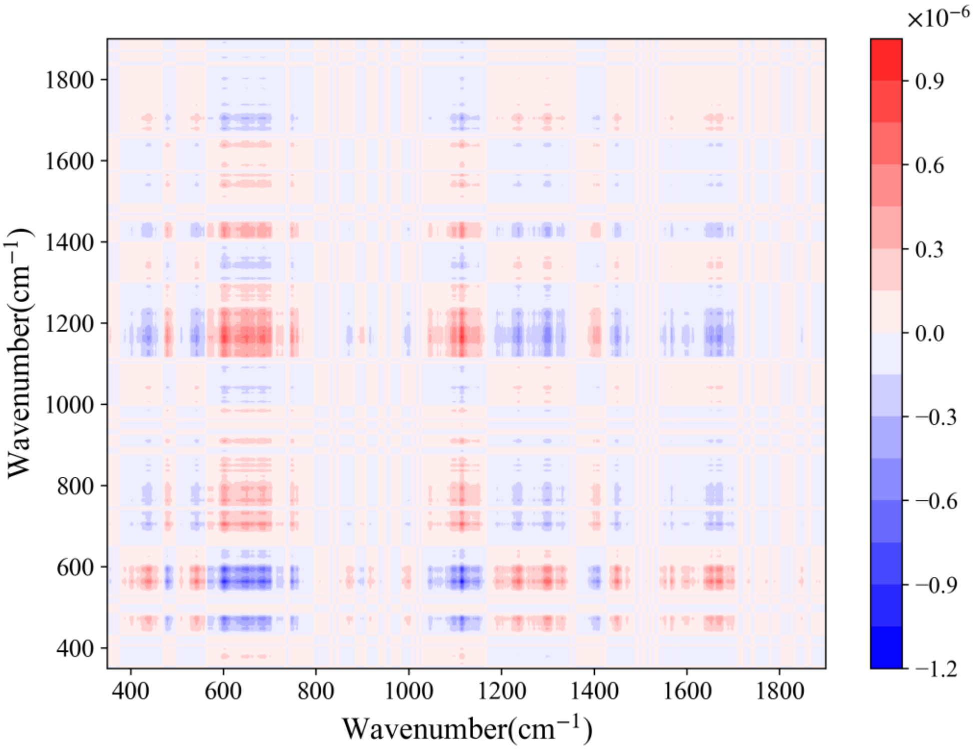

Figure 3. asynchronous 2D correlation spectra

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Poster (P18)

APPLICATION OF COMPOSITE MATERIALS IN THE REMEDIATION OF EMERGING CONTAMINANTS

Ziyi Wu, Yuhai Liu

College of Ecology and Environment, Hainan University

Antibiotic pollution in aquatic environments primarily originates from domestic sewage, medical wastewater, and aquaculture effluent. Residues can promote the proliferation and spread of antibiotic resistance genes (ARGs), threatening ecosystems and human health. Sulfonamides (SAs), one of the most extensively used classes of veterinary drugs globally, are consumed in China in quantities exceeding the rest of the world combined.

Adsorption using modified biochar is one of the most prevalent and mature remediation technologies. Synthesizing novel modified biochar holds significant importance.

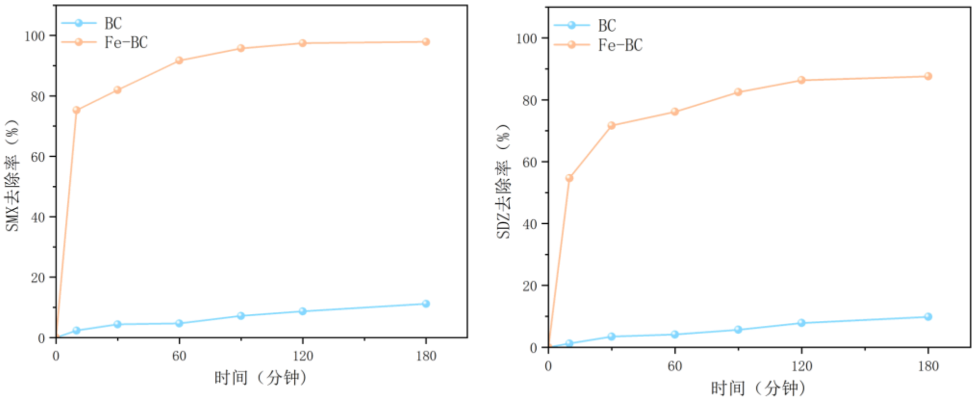

Figure 1. Effect of contact time on the adsorption of sulfonamides by Fe-BC and BC

The iron and nitrogen co-doped biochar (Fe-N-BC), prepared via pyrolysis, exhibited significantly enhanced removal performance for sulfamethoxazole (SMX). As shown in Figure 1, Fe-N-BC achieved a 90% removal rate for SMX within 3 hours, an increase of 75 percentage points compared to the unmodified biochar (BC). This enhanced adsorption capacity primarily stems from two factors: (1) Optimized physicochemical structure: Fe-N-BC exhibits a larger specific surface area (BET), a more developed porous structure, and loaded iron oxides, which provides abundant adsorption sites and enhances removal via Fe-SMX coordination. (2) Dominant interaction forces: π-π electron donor-acceptor (EDA) interactions and hydrogen bonding were identified as the core mechanisms governing SMX adsorption.