### **BUKTI KORESPONDENSI**

# ARTIKEL PROSEDING TERINDEKS SCOPUS

Judul Artikel : Water Quality in the Maintenance of Oreochromis niloticus through

Environmentally Friendly Biofloc Technology

Nama Seminar: ICDM 2019

Judul Proseding: IOP Conference Series: Materials Science and Engineering, ICDM 2019,

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Pelaksanaan : Grand Candi Hotel Semarang, 2-4 September 2019

Penulis : Endah Rita Sulistya Dewi, Ary Susatyo Nugroho, Maria Ulfah

No.	Perihal	Tanggal
1.	Bukti konfirmasi submit Abstrak	18 Juli 2019
2.	Konfirmasi Abstrak di setujui	24 Juli 2019
3.	Bukti Pembayaran	22 Agustus 2019
4.	Bukti Upload Full Paper	26 Agustus 2019
5.	Bukti Undangan untuk presentasi pada seminar ICDM 2019	30 Agustus 2019
6.	Bukti konfirmasi artikel published online	1 Mei 2020

## Submit Article ICDM

Dari: Endah RIta Sulistya Dewi (endahrita@yahoo.co.id)

Kepada: icdm@upgris.ac.id

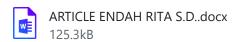
Tanggal: Kamis, 18 Juli 2019 10.20 GMT+7

### Dear team editor ICDM

I have submitted my article about Water Quality in the Maintenance of Oreochromis niloticus through Environmentally Friendly Biofloc Technology, Hopefully it will get a response and be published soon.thank you very much

# Regards

Endah Rita Sulistya Dewi Universitas PGRI Semarang, Indonesia



# [ABS-63] Abstract Edited

Dari: ICDM 2019 (icdm@upgris.ac.id)

Kepada: endahrita@yahoo.co.id

Tanggal: Selasa, 24 Juli 2018 14.24 GMT+7

Dear Dr. Endah Rita Sulistya Dewi,

Your abstract:

Abstract ID:

ABS-63

Please use this "Abstract ID" in all correspondence (instead of abstract title).

Title:

Water Quality in the Maintenance of Oreochromis niloticus through Environmentally Friendly Biofloc Technology

Authors:

Endah Rita Sulistya Dewi, Ary Susatyo Nugroho, Maria Ulfah

Institutions:

Departement of Mathematics, Sciences and Information Technology, PGRI Semarang University, Indonesia Jl. Sidodadi Timur No. 24 Semarang Indonesia 50125 email:endahrita@yahoo.co.id

#### Content:

This Population growth that continues to increase demands continuous availability of food. Aquaculture is one of the sectors of food production which has the highest growth rate in the world. Facing this opportunity, aquaculture is faced with several challenges related to limited natural resources such as water and land, as well as waste water from aquaculture. Furthermore, the application of best aquaculture practices in aquaculture product certification requires environmentally friendly aquaculture practices. Oreochromis niloticus tilapia is a type of freshwater consumption fish and is now a popular pet fish in freshwater ponds in Indonesia. This study aims to analyze water quality in the maintenance of Tilapia through environmentally friendly Biofloc technology. This research method was designed in the form of Research and Development. The results showed that the water quality was proper for pond operation using minimal water exchange, the development of dense microbial populations through the management of microbial populations could control the concentration of ammonia in the water. Bacteria in ponds form biofloc, producing microbial proteins that make it possible to recycle unused feed protein, so as to minimize pollution.

Keywords:

Biofloc, Oreochromis niloticus, Environment Friendly

Topic: Science

Presenter:

Endah Rita Sulistya Dewi

Type:

**Oral Presentation** 

The Letter of Acceptance (LoA) can be downloaded from your account, once your abstract is accepted to be presented.

Thank you.

Best Regards,

ICDM 2019 Organizing Committee Website: <a href="http://icdm.upgris.ac.id">http://icdm.upgris.ac.id</a> Email: <a href="mailto:icdm@upgris.ac.id">icdm@upgris.ac.id</a>

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Automated Conference System provided by Konfrenzi | <a href="http://konfrenzi.com">http://konfrenzi.com</a>

# Announcement

Dari: ICDM (icdm@upgris.ac.id)

Kepada: endahrita@yahoo.co.id

Tanggal: Rabu, 14 Agustus 2019 14.54 GMT+7

### Dear Presenters,

Your abstract has been reviewed. Please kindly login to your account to check whether your abstract should be revised or not. Then the next step is uploading the receipt of presenters' payment. The last please upload the full paper.

# Regard, Admin of ICDM

### Announcement

Dari: ICDM (icdm@upgris.ac.id)

Bcc: endahrita@yahoo.co.id

Tanggal: Kamis, 22 Agustus 2019 13.36 GMT+7

### Dears presenters,

Please, kindly login to your account to upload your payment receipt and full paper no late than August 30, 2019.

The details of payment are: First Author: **Rp. 2.500.000,-**

For further information please contact:

## **Admin ICDM**

Mega Novita (0819 5899 0880)

# [ABS-63 FULL\_PAPER] File Submitted to ICDM 2019

Dari: ICDM (icdm@upgris.ac.id)
Kepada: endahrita@yahoo.co.id

Tanggal: Kamis, 22 Agustus 2019 12.13 GMT+7

Dear Dr. Endah Rita Sulistya Dewi,

We have received the submission of your file.

Abstract ID: ABS-63

Title

Water Quality in the Maintenance of Oreochromis niloticus through Environmentally Friendly Biofloc Technology

Authors:

Endah Rita Sulistya Dewi, Ary Susatyo Nugroho, Maria Ulfah

Type: full\_paper

Topic: Science

Presenter:

Endah Rita Sulistya Dewi

Thank you very much.

Best Regards,

ICDM 2019 Organizing Committee Website: http://icdm.upgris.ac.id Email: icdm@upgris.ac.id

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# [ABS-63 PAYMENT\_PROOF] File Submitted to ICDM 2019

Dari: ICDM (icdm@upgris.ac.id)
Kepada: endahrita@yahoo.co.id

Tanggal: Senin, 26 Agustus 2019 12.33 GMT+7

Dear Dr. Endah Rita Sulistya Dewi,

We have received the submission of your file.

Abstract ID: ABS-63

Title:

Water Quality in the Maintenance of Oreochromis niloticus through Environmentally Friendly Biofloc Technology

Authors:

Endah Rita Sulistya Dewi, Ary Susatyo Nugroho, Maria Ulfah

Type:

payment\_proof

Paid amount: IDR 2500000

Transfer date: 2018.08.22

Topic: Science

Presenter:

Endah Rita Sulistya Dewi

The Payment Receipt can be downloaded directly from your account, once your payment has been confirmed.

Thank you.

Best Regards,

ICDM 2019 Organizing Committee Website: http://icdm.upgris.ac.id Email: icdm@upgris.ac.id

\_\_\_\_\_

Listed in Indonesia Conference Directory | http://ifory.net Automated Conference System provided by Konfrenzi | http://konfrenzi.com

#### Announcement

Dari: ICDM (icdm@upgris.ac.id)

Bcc: endahrita@yahoo.co.id

Tanggal: Jum'at, 30 Agustus 2019 15.43 GMT+7

Dear Presenters of the ICDM 2019,

We hope this email finds you well. We would like to inform you the rundown of ICDM 2019 and the parallel session distribution. Please kindly attach the attachment below. To add, the presentation will be done not more than 7 minutes.

Please do not hesitate to contact us for more information \*Mega Novita (0819 5899 0880)

with best regards, Your the ICDM 2019 Organizers





# **PROGRAM BOOK**

# In the 7th International Conference on DV-Xa Method

The Advances-Related Experiments and Theories on Material Science Universitas PGRI Semarang, Central Java, Indonesia 2-4 September 2019

Co-host















#### **Welcome Remarks:**

**Conference Chairperson ICDM 2019** 



Mega Novita, S.Si., M.Si., M.Nat.Sc., Ph.D

It is a great honour and pleasure to welcome you at the  $7^{th}$  International Conference on DV-X $\alpha$  Method: The Advances-Related Experiments and Theories on Material Science (ICDM 2019). We are happy to have you from 2 - 4 September 2019 in Semarang. This event is organized by Universitas PGRI Semarang (UPGRIS - Indonesia) in cooperation with DV-Xa Society (Japan), Kwansei Gakuin University (Japan), Kobe University (Japan), Universitas 17 Agustus 1945 Semarang (Indonesia), Universitas PGRI Madiun (Indonesia) and under the coordination of Centre of Science and Technology UPGRIS (Indonesia).

ICDM is an international event aimed at presenting contemporary research and accommodating discussion for scientists, scholars, engineers, students, research institutes, and industries in the field of advanced materials, science and information technology.

The interaction between the theoretical and practical aspects of integrating the innovative and advanced technologies would construct new fundamentals in the engineering field. Therefore, it would be one direction that ICDM should pursue, hence the theme of our symposium is "The Advances-related experiments and theories on material science".

We would like to express our gratitude to all keynote and invited speakers, and all participants who have travelled far away. Our appreciation also goes to the committee members who have worked hard to make this event possible. Thus, we wish all participants may engage in the fruitful and meaningful discussion in this conference.

# Welcome Remarks:















#### **Rector, Universitas PGRI Semarang**



Dr. Muhdi, S.H., M.Hum

I would like to warmly welcome you all to Semarang, Indonesia.

It is an honour for Universitas PGRI Semarang (UPGRIS-Indonesia) to be the host of the  $7^{th}$  International Conference on DV-X $\alpha$  Method: The Advances-Related Experiments and Theories on Material Science (ICDM 2019). We are pleased to have cooperation with DV-X $\alpha$  Society to hold this international event. As we know, the previous conferences related to this topic had been conducted six times: once in Hungary, three times in South Korea, two times in Japan and supported by some institutions as the hosts: The Institute of Nuclear Research of the Hungarian Academy of Sciences (ATOMKI-Hungary), Seoul National University (South Korea), Kunsan National University (South Korea), National Institute of Physical and Chemical Research (RIKEN-Japan), Korean Basic Science Institute (KBSI-South Korea), and University of Hyogo (Japan).

Therefore, we expect that the cooperation in running the event will be successful in the implementation. We also proudly invited Kwansei Gakuin University (KGU-Japan), Kobe University (Japan), Universitas PGRI Madiun (UNIPMA-Indonesia) and Universitas 17 Agustus 1945 (UNTAG-Indonesia) to be the co-hosts of the conference.

We would like to express our sincere gratitude and appreciation to all parties for any fatigue and support in organizing this event. Furthermore, we expect that this conference can facilitate researchers, engineers,

lecturers, academicians and practitioners to discuss and collaborate. We hope that this conference have positive impacts to strengthen and foster international networks and publications related to this field and















particularly introduce DV-X $\alpha$  method in Indonesia. Herewith, we are pleased to share the latest development of the powerful method to analyse advanced materials, science and IT through DV-X $\alpha$  method.

Eventually, I sincerely hope that this conference may bring benefits for all of us.

Thank you















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# **GENERAL CONFERENCE PROGRAM**

Conference Day 1: September 2, 2019	
08:00-09:00	Registration
09:00-09:15	Welcoming Speech Mega Novita, S.Si., M.Si., M.Nat.Sc., Ph.D (Chairperson of ICDM 2019, Universitas PGRI Semarang, Indonesia)
09:15-11:00	Lecture Session 1 Moderator: Prof. Jun Onoe (Nagoya University, Japan)
09:15-10:00	ABS-5 (Keynote Speaker) Supramolecular Rare Sugar Prof. Tomohiko Ishii Kagawa University, Japan
10:00-10:15	Coffee Break
10:15-11:00	ABS-42 (Keynote Speaker)  Microscopic crystal field effects in impurity centers formed by the transition metal ions  Prof. Mikhail G. Brik  University of Tartu, Estonia
11:00-12:00	Lecture Session 2 Moderator: Dr. Retno Ambarwati (Universitas 17 Agustus 1945 Semarang Indonesia)
11:00-11:20	ABS-3 (Invited Speaker)  Sorption characteristics of ferrocyanide nanoparticles to metal ions in nitric acid solution for development of vitrification processes of high level radioactive nuclear wastes  J. Onoe <sup>1</sup> , S. Watanabe <sup>1</sup> , M. Harigai <sup>2</sup> , Y. Inaba <sup>2</sup> , and K. Takeshita <sup>2</sup> <sup>1</sup> Nagoya University, <sup>2</sup> Tokyo Inst. Technol., Japan















	ADG 40 (T. 1/4 LG. L.)
	ABS-29 (Invited Speaker)
	Week Hydrogen Bonding of Polymers Studied by Terahertz
11:20-11:40	and Low-frequency Raman Spectroscopy
	Prof. Harumi Sato
	Kobe University, Japan
	ABS-35 (Invited Speaker)
	Recent applications of discrete variational multi-electron
11:40-12:00	method
	Prof. Kazuyoshi Ogasawara
	Kwansei Gakuin University, Japan
12:00-13:00	Lunch Break
	Poster Session (3 Minutes Presentation)
13:00-14:45	Moderator: Dr. Dyah Nugrahani (Universitas PGRI
	Semarang, Indonesia)
	ABS-4
	Crystal Size Effect in Polaritonic Luminescence from
	Atomic Cryocrystals
	Alexander Ogurtsov, Olga Bliznjuk, Nataliia Masalitina
	National Technical University "KhPI"
	Ukraine
	ABS-9
	Prediction of $4f2\rightarrow 4f15d1$ transition energy of Pr3+ in
	fluorides based on first-principles calculations and machine
	learning
	Hayato Obata, Kazuyoshi Ogasawara
	Kwansei Gakuin University, Japan
	ABS-10
	Optimization of first-principles calculation conditions of
	multiplet energies in Fe3 + and Co3 + in $\alpha$ -Al2O3
	Judo Fusamoto, Kazuyoshi Ogasawara
	Kwansei Gakuin University, Japan
	ABS-12
	Prediction of 4f7→4f65d1 transition energies of Eu2+ in
	oxides based on first-principles calculations and machine
	learning
	Hiroyuki Hori, Shota Takemura, Kazuyoshi Ogasawara
	Kwansei Gakuin University, Japan















ABS-18
Controlling of the Spin State by Jahn-Teller Distortion in
Octahedral Hexa- Coordinate Metal Complex
T. Oguma, Y. Huzikawa, D. Tsuneda, Y. Tsutsumi, M.
Nakano, T. Ishii, G. Sakane,
Kagawa University, Japan
ABS-19
Single-Crystal X-Ray Structural Analysis and Electronic
Structures Calculation of Rare Sugar
Bui Quoc Huy, Tomohiko Ishii, Norito Taniguchi, Natsumi
Nagayama, Genta Sakane
Kagawa University, Japan
ABS-22
Prediction of emission energy of Cr3+ in oxides based on
first-principles calculations and machine learning
Tsubasa Hori, Kazuyoshi Ogasawara
Kwansei Gakuin University, Japan
ABS-23
Consideration of Super Atomic Hibrid Orbital in Super
Atom $M@Al12$ ( $M = Be, Mg, Ca, Sr$ )
Teruyuki Toba, Ishii Tomohiko, Syoya Yamasaki, Sakane
Genta
Kagawa University, Japan
ABS-24
Mechanism of Optical Rotation of Amino Acids Using
Electronic State Calculation
Shuuichi Katumoto, Manami Mimura, Tomohiko Ishii, and
Genta Sakane
Kagawa University, Japan
ABS-25
Generation of Two-Dimensional Spectrochemical Series in
Tetrahedral Complexes
Takuhiro Yamamoto, Takeyoshi Oguma, Momoe Nakano,
Akira Tsuneda, Yuki Tsutsumi, Tomohiko Ishii
Kagawa University, Japan
ABS-26
Effect of Molecular Distortion of Ligand Field Splitting in
Five-Coordinated Metal Complex















	X 1 '1 ' D ''1
	Yohiki Fujikawa, Takeyoshi Oguma, Takuhiro Yamamoto,
	Yuki Tsutsumi, Dan Tsuneda, Momoe Nakano, Tomohiko
	Ishii, Genta Sakane
	Kagawa University, Japan
	ABS-27
	Single crystal X-ray structural analysis of sugar molecules
	and electronic theory
	Norito TANIGUCHI, Tomohiko ISHII, Bui Quoc Huy,
	Natsumi NAGAYAMA, Genta SAKANE
	Kagawa University, Japan
	ABS-31
	Contribution of edge-carbon atoms and non-benzenoid
	rings in graphitic carbons to π* peak profiles in CK-XANES
	Yasuji Muramatsu and Yuma Hirai
	University of Hyogo, Japan
	ABS-48
	Designing Enterprise Architecture in Koperasi Karyawan
	using TOGAF Architecture Development Method
	Noora Qotrun Nada, Setyoningsih Wibowo, Mega Novita
	Universitas PGRI Semarang, Indonesia
	ABS-49
	ABS-49 DECISION SUPPORT SYSTEM MUSEUM AMBASSADOR
	ABS-49 DECISION SUPPORT SYSTEM MUSEUM AMBASSADOR USING TOPSIS METHOD
	ABS-49 DECISION SUPPORT SYSTEM MUSEUM AMBASSADOR USING TOPSIS METHOD Setyoningsih Wibowo, Maichifa Ayuning Tyas, Noora
	ABS-49 DECISION SUPPORT SYSTEM MUSEUM AMBASSADOR USING TOPSIS METHOD Setyoningsih Wibowo, Maichifa Ayuning Tyas, Noora Qotrun Nada, Mega Novita
	ABS-49 DECISION SUPPORT SYSTEM MUSEUM AMBASSADOR USING TOPSIS METHOD Setyoningsih Wibowo, Maichifa Ayuning Tyas, Noora Qotrun Nada, Mega Novita Universitas PGRI Semarang, Indonesia
	ABS-49 DECISION SUPPORT SYSTEM MUSEUM AMBASSADOR USING TOPSIS METHOD Setyoningsih Wibowo, Maichifa Ayuning Tyas, Noora Qotrun Nada, Mega Novita
	ABS-49 DECISION SUPPORT SYSTEM MUSEUM AMBASSADOR USING TOPSIS METHOD Setyoningsih Wibowo, Maichifa Ayuning Tyas, Noora Qotrun Nada, Mega Novita Universitas PGRI Semarang, Indonesia
	ABS-49 DECISION SUPPORT SYSTEM MUSEUM AMBASSADOR USING TOPSIS METHOD Setyoningsih Wibowo, Maichifa Ayuning Tyas, Noora Qotrun Nada, Mega Novita Universitas PGRI Semarang, Indonesia ABS-50
	ABS-49 DECISION SUPPORT SYSTEM MUSEUM AMBASSADOR USING TOPSIS METHOD Setyoningsih Wibowo, Maichifa Ayuning Tyas, Noora Qotrun Nada, Mega Novita Universitas PGRI Semarang, Indonesia ABS-50 Design of Augmented Reality Game app "IntroME" using
	ABS-49 DECISION SUPPORT SYSTEM MUSEUM AMBASSADOR USING TOPSIS METHOD Setyoningsih Wibowo, Maichifa Ayuning Tyas, Noora Qotrun Nada, Mega Novita Universitas PGRI Semarang, Indonesia ABS-50 Design of Augmented Reality Game app "IntroME" using ADDIE Model
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	ABS-49 DECISION SUPPORT SYSTEM MUSEUM AMBASSADOR USING TOPSIS METHOD Setyoningsih Wibowo, Maichifa Ayuning Tyas, Noora Qotrun Nada, Mega Novita Universitas PGRI Semarang, Indonesia ABS-50 Design of Augmented Reality Game app "IntroME" using ADDIE Model Rahmat Robi Waliyansyah, Irfan Nur Ridwan, Khoirul Huda, Febrian Murti Dewanto Universitas PGRI Semarang, Indonesia ABS-53 DESIGNING ANDROID BASED EDUCATION GAME
	ABS-49 DECISION SUPPORT SYSTEM MUSEUM AMBASSADOR USING TOPSIS METHOD Setyoningsih Wibowo, Maichifa Ayuning Tyas, Noora Qotrun Nada, Mega Novita Universitas PGRI Semarang, Indonesia ABS-50 Design of Augmented Reality Game app "IntroME" using ADDIE Model Rahmat Robi Waliyansyah, Irfan Nur Ridwan, Khoirul Huda, Febrian Murti Dewanto Universitas PGRI Semarang, Indonesia ABS-53 DESIGNING ANDROID BASED EDUCATION GAME AKSARA JAWA USING SHUFFLE RANDOM ALGORITHM
	ABS-49 DECISION SUPPORT SYSTEM MUSEUM AMBASSADOR USING TOPSIS METHOD Setyoningsih Wibowo, Maichifa Ayuning Tyas, Noora Qotrun Nada, Mega Novita Universitas PGRI Semarang, Indonesia ABS-50 Design of Augmented Reality Game app "IntroME" using ADDIE Model Rahmat Robi Waliyansyah, Irfan Nur Ridwan, Khoirul Huda, Febrian Murti Dewanto Universitas PGRI Semarang, Indonesia ABS-53 DESIGNING ANDROID BASED EDUCATION GAME AKSARA JAWA USING SHUFFLE RANDOM
	ABS-49 DECISION SUPPORT SYSTEM MUSEUM AMBASSADOR USING TOPSIS METHOD Setyoningsih Wibowo, Maichifa Ayuning Tyas, Noora Qotrun Nada, Mega Novita Universitas PGRI Semarang, Indonesia  ABS-50 Design of Augmented Reality Game app "IntroME" using ADDIE Model Rahmat Robi Waliyansyah, Irfan Nur Ridwan, Khoirul Huda, Febrian Murti Dewanto Universitas PGRI Semarang, Indonesia  ABS-53 DESIGNING ANDROID BASED EDUCATION GAME AKSARA JAWA USING SHUFFLE RANDOM ALGORITHM Nugroho Dwi Saputro, Tri Ana Romadhani, Febrian Murti Dewanto
14:45-15:00	ABS-49 DECISION SUPPORT SYSTEM MUSEUM AMBASSADOR USING TOPSIS METHOD Setyoningsih Wibowo, Maichifa Ayuning Tyas, Noora Qotrun Nada, Mega Novita Universitas PGRI Semarang, Indonesia  ABS-50 Design of Augmented Reality Game app "IntroME" using ADDIE Model Rahmat Robi Waliyansyah, Irfan Nur Ridwan, Khoirul Huda, Febrian Murti Dewanto Universitas PGRI Semarang, Indonesia  ABS-53 DESIGNING ANDROID BASED EDUCATION GAME AKSARA JAWA USING SHUFFLE RANDOM ALGORITHM Nugroho Dwi Saputro, Tri Ana Romadhani, Febrian Murti















	<u>,                                      </u>
15:00-16:30	Lecture Session 3
	Moderator: Prof. Yasuji Muramatsu (University of Hyogo,
	Japan)
15:00-15:45	ABS-6 (Keynote Speaker)
	X-ray Absorption Spectroscopy and Its Simulation for Some
	Metal Oxides
	Prof. Deok-Yong Cho
	Chonbuk National University, South Korea
15:45-16:30	ABS-46 (Keynote Speaker)
	Carotenoid Dynamics Free and Bound to Pigment Protein
	Complexes: The Role of the 11Bu- State
	Prof. Ferdy Samuel Rondonuwu
	Satya Wacana Christian University, Indonesia
16:30-17:30	Lecture Session 4
	Moderator: Asst. Prof. Laily Nur Affini
16:30-16:50	ABS-30 (Invited Speaker)
	Metal complexes with sulfur-containing ligands
	Masahiro Mikuriya and Makoto Handa
	Kwansei Gakuin University, Japan
16:50-17:10	ABS-54 (Invited Speaker)
	Electronic state of sulfide-based alkali-ion conducting
	solid-state electrolytes applied to all-solid-state secondary
	batteries
	Yoshiyuki Kowada, Yasukazu Akaki, Akiotoshi Hayashi,
	and Masahiro Tatsumisago
	Hyogo University of Teacher Education, Japan
17:10-17:30	ABS-55 (Invited Speaker)
	Geometry and Stability of Small Gold Cluster Ions by
	Graph Theory and Hückel model
	Rika Sekine, Takashi Kasai, Eri Furuta, and Masaya
	Okakura
	Shizuoka University, Japan
17:30-19:00	Break
19:00-21:00	Gala dinner













Conference Day 2: September 3, 2019	
Parallel room 1	
08:00-10:00	Moderator: Prof. Masataka Mizuno (Osaka University,
	Japan)
	Asst. Moderator: Asst. Prof. Laily Nur Afini (Universitas
	PGRI Semarang, Indonesia)
	ABS-1 (Invited Speaker)
08:00-08:20	First-Principles Calculation of Laser Crystal Multiplet
	Levels via Hybridized Density Functional Theory and
00.00-00.20	Configuration Interaction within the OLCAO Method
	Dr. Benjamin Walker
	University of Missouri - Kansas City, USA
	ABS-8 (Invited Speaker)
	Systematic First-Principles Calculations of Charge
	Transfer Transitions of Transition Metal Ions (Sc3+, Ti3+,
08:20-08:40	$V3+$ , $Cr3+$ , $Mn3+$ , $Fe3+$ ) in $\alpha$ -Al2O3 with Structural
	Optimization
	Shota Takemura1, Mega Novita2, Kazuyoshi Ogasawara1
	Kwansei Gakuin University, Japan
	ABS-16 (Invited Speaker)
	Study of LCAO-MO calculation by using completely
08:40-09:00	numerical basis functions
	Katsumi Nakagawa
	MO Basics Research
	ABS-13
	Lattice Relaxation Effects on the Multiplet Energies of Ruby
09:00-09:15	Under Pressure using One-Electron Calculations
	Mega Novita, Nur Cholifah, Kazuyoshi Ogasawara
	Universitas PGRI Semarang, Indonesia, Kwansei Gakui
	University, Japan ABS-14
	Optical properties of Co3+ doped in α-Al2O3 with Considering Lattice Relaxation Effect
09:15-09:30	Mega Novita, Duwi Nuvitalia, Nur Cholifah, Kazuyoshi
09.13-09.30	
	Ogasawara Universitas PGRI Semarang, Indonesia, Kwansei Gakui
	University, Japan
	ABS-15
09:30-09:45	Effects of Transition Metal Doping to Cerium-Oxides in
07.30-07.43	Thermal Reduction Reaction
L	тистим Кешисион Кешсион















	Takaki Nishimura, Yuki Tsutsumi, Tomohiko Ishii, Tatsuya
	Kodama, and Genta Sakane
	Kagawa University, Japan
	ABS-61
00 47 10 00	Extraction Sentiment Analysis Using Naive Bayes Algorithm
09:45-10:00	and Reducing Noise Word Applied in Indonesian Language
	Aris Tri Jaka Harjanta, Bambang Agus Herlambang
	Universitas PGRI Semarang, Indonesia
00 00 10 00	Parallel room 2
08:00-10:00	Moderator: Prof. Prompong Pienpinijtham (Chulalongkom
	University Thailand)
	Asst. Moderator: Dr. Muchamad Taufiq Anwar (Universitas
00.00.00.00	Stikubank, Indonesia)
08:00-08:20	ABS-2 (Invited Speaker)
	Soil decontamination by cesium-free mineralization with
	CaCl2: effect of chlorine on phase transformation of a clay
	mineral
	Iwao Shimoyama
	Japan Atomic Energy Agency, Japan
08:20-08:40	ABS-7 (Invited Speaker)
	Study on The Higher-Order Structure and Hydrogen
	Bonding of Biodegradable Polymer by Low-Frequency
	Vibrational Spectroscopy
	Dian Marlina, Harumi Sato
	Kobe University, Japan
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	An elaborate response in molecular random network -
	Approach for information processing functionality-
	Megumi Akai-Kasaya
00.00.00.17	Osaka University, Japan
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	Cultivation of Oreochromis niloticus with an
	Environmentally friendly Bioflog System
	Endah Rita Sulistya Dewi, Ary Susatyo Nugroho, Maria
	Ulfah
	Universitas PGRI Semarang, Indonesia















r	
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	Data Mining Application with Fuzzy Logic Method for
	Monitoring Vehicle Position Based on Android
	Munaf Ismail, Sri Arttini Dwi Prasetyowati, Ida Widihastuti
	Universitas Islam Sultan Agung, Indonesia
09:30-09:45	ABS-33
	Smart Aquaponics Design Using Internet of Things
	Technology
	R Hafid Hardyanto, Prahenusa Wahyu Ciptadi
	Universitas PGRI Yogyakarta, Indonesia
09:45-10:00	ABS-36
	Alternative Solutions For Determining Village Funds Using
	Weight Product Method
	Tri Hastono, Firdiyan Syah
	Universitas PGRI Yogyakarta, Indonesia
10:00-10.15	Coffee Break
10:00-10:30	Preparation
10:30-12:30	Heading to Candi Borobudur
12:30-13:30	Lunch
13:30-18:00	Excursion
18:00-19:00	Dinner
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Conference Day 3: September 4, 2019	
08:00-10:45	Parallel room 1
00.00 10.15	Moderator: Prof. Katsumi Nakagawa (MO Basic Research,
	Japan)
	Asst. Moderator: Dr. Dyah Nugrahani (Universitas PGRI
	Semarang, Indonesia)
08:00-08:20	ABS-34 (Invited Speaker)
	Stability of carbon-vacancy complexes in α-Fe
	Masataka Mizuno, Waka Yamada, Kazuki Sugita, Hideki
	Araki
	Osaka University, Japan
08:20-08:40	ABS-37 (Invited Speaker)
	DESIGN OF ELECTRICITY ENERGY SOURCES IN
	SEMARANG PGRI UNIVERSITY USING OFF-GRID
	SOLAR PANEL SYSTEMS
	Adhi Kusmantoro, Mega Novita, Th.Indriati Wardani
	Universitas PGRI Semarang, Indonesia
08:40-09:00	ABS-38 (Invited Speaker)
	Novel shape analysis method for single bioparticles in
	aqueous solutions
	Sou Ryuzaki, Makusu Tsutsui, Masateru Taniguchi
	Kyushu University, Japan
09:00-09:15	Coffee break
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	BIOCONVERSION ON WASTEWATER OF SOYBEAN
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09:15-09:30	Yohanes A Cahyono, Tilana Madurani, Widya F Azzahra
	and Retno A. S. Lestari
09:30-09:45	Universitas 17 Agustus 1945 Semarang, Indonesia  ABS-44
09:30-09:43	Potential of Ketapang Seed Oil (Terminalia catappa Linn)
	as Basic Material Mono-diglyceride Biodegradable
	Surfactant
	Ery Fatarina Purwaningtyas, Khoir Fadilah
	Universitas 17 Agustus 1945 Semarang, Indonesia
09:45-10:00	ABS-45
252 20.00	BIOPLASTIC FROM JACKFRUIT SEEDS AND RICE
	WASTE
	Retno A.S. Lestari, Mega Kasmiyatun, Kevin Dermawan,
	Alfia N. Aini, Nur Riyati, Finka R. Putri















	Universitas 17 Agustus 1945 Semarang, Indonesia
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10.00 10.13	The Multi-agents System for Job Recommender System
	Meilany Nonsi Tentua, Azhari SN, Aina Musdholifah
	Universitas PGRI Yogyakarta, Indonesia
10:15-10:30	ABS-62
10.13 10.30	The Effect Of Decomposer Microorganism Additions On
	The Natural Hydroponic Technology (Nht) Systems Of
	Pakcoi Growth
	Ary Susatyo Nugroho $^{\overline{1}}$ , Endah Rita S. Dewi $^{\overline{2}}$ , M. Anas
	Dzakiy <sup>3</sup>
	Program Studi Pendidikan Biologi FPMIPATI Universitas
	PGRI Semarang
10:30-10:45	ABS-58
	Interaction Analysis Application of Arduino Industrial
	Automation Trainer Based on Project to Improve Cognitive
	Ability and Bodily Kinesthetic Ability
	Ir. Sulistyaning Kartikawati, MM, M.Pd., Sekreningsih
	Nita, S.Kom, MT.
	Universitas PGRI Madiun, Indonesia
08:00-10:45	Parallel room 2
	Moderator: Dr. Benjamin Walker (University of Missouri -
	Kansas City)
	Asst. Moderator: Dr. Dian Marlina (Kobe University,
00.00.00.20	Japan)
08:00-08:20	ABS-28 (Invited Speaker)
	Structural changes in graphene oxide induced by silver
	nanoparticles – TERS study
	Prompong Pienpinijtham, Sanpon Vantasin, Oraporn Wongura, Yasutaka Kitahama, Sanong Ekgasit and Yukihiro
	Ozaki
	Chulalongkom University Thailand
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	(MgNH4PO4.6H2O): From basic research to applications
	Stefanus Muryanto
	Universitas 17 Agustus 1945 Semarang, Indonesia
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	THE EFFECT OF CHLORIDE ACID (HCL)
	CONCENTRATION AND FERMENTATION ON















	DIOETHANOL LEVELS EDOM DDEADEDIUT (Auto-common
	BIOETHANOL LEVELS FROM BREADFRUIT (Artocarpus
	Artilis) SUBSTRATE
	Nasrul Rofiah Hidayati
00.00.00.15	Universitas PGRI Madiun
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	Design of Product Monitoring System using Internet of
	Things Technology for Smart Manufacturing
	Marti Widya Sari, Herianto, IGB Budi Dharma, Alva Edy
	Tontowi
	Universitas PGRI Yogyakarta, Indonesia
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	A Novel and Fast Memory Perturbation Method to Increase
	Exploration in Particle Swarm Optimization Algorithm
	Eri Zuliarso, Muchamad Taufiq Anwar, Kristophorus
	Hadiono, Iswatun ChasanahUniversitas Stikubank,
	Indonesia
09:45-10:00	ABS-43
	Internet of Things (IOT) with Cloud Computing and
	Machine to Machine (M2M) communication in Aquaponics
	Farming Systems
	Prahenusa Wahyu Cipadi, R.Hafid Hardyanto
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	Detecting Hoaxes in Indonesian News Using TF-IDF and K
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	Muchamad Taufiq Anwar, Edy Winarno, Iswatun Chasanah
	Universitas Stikubank, Indonesia
10:15-10:30	ABS-59
	ANALYSIS OF THE IMPACT NARRATIVE ALGORITHM
	METHOD, PSEUDOCODE AND FLOWCHART
	TOWARDS STUDENTS UNDERSTANDING OF THE
	PROGRAMMING ALGORITHM COURSES
	Sekreningsih Nita, Sulistyaning Kartikawati
	Universitas PGRI Madiun, Indonesia
10:30-10:45	ABS-60
23.23 23.13	Prediction of The Number Job Seeker Using
	Backpropagation Neural Network Method
	Khoiriya Latifah, Agung Handayanto, Anita Rahayu
	Universitas PGRI Semarang, Indonesia
	Omversitus i OKI belliarang, muonesia















10:45-11:00	Coffee break		
11:00-12:00	Closing Ceremony Moderator: Dr. Dyah Nugrahani (Universitas PGRI Semarang, Indonesia)		
11:00-11:35	DV-Xα meeting Prof. Yoshiyuki Kowada (Hyogo University of Teacher Education, Japan)		
11:35-11:55	Awards Prof. Katsumi Nakagawa (MO Basic Research, Japan)		
11:55-12:00	Closing statement Mega Novita, S.Si., M.Si., M.Nat.Sc., Ph.D (Chairperson of ICDM 2019, Universitas PGRI Semarang, Indonesia)		
12:00-13:00	Lunch		















#### LECTURE SESSIONS TIMETABLE

# The 7<sup>th</sup> International Conference on DV-Xα Method (ICDM 2019) Grand Candi Hotel, Semarang, INDONESIA 2-4 September 2019

	2-Sep-2019		3-Sep-2019		4-Sep	-2019
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09:00-09:15	Welcoming Speech	08:20-08:40	ABS-8	ABS-7	ABS-37	ABS-51
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12:00-13:00	Lunch Break	10:15-10:30			ABS-62	ABS-59
13:00-14:45	Poster session	10:30-10:45			ABS-58	ABS-60
14:45-15:00	Coffee break	10:45-11:00			Coffee	break
15:00-15:45	ABS-6	11:00-11:35			DV-Xα gen	eral meeting
15:45-16:30	ABS-46	11:35-11:55			Aw	ards
16:30-16:50	ABS-30	11:55-12:00			Closing s	statement
16:50-17:10	ABS-54	12:00-13:00	]		Lui	nch
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19:00-21:00





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### ABS-1 First-Principles Calculation of Laser Crystal Multiplet Levels via Hybridized Density Functional Theory and Configuration Interaction within the OLCAO Method

Dr. Benjamin Walker

University of Missouri - Kansas City

Computation of highly-localized multiplet energy levels of transition metal dopants is essential to the design of materials such as laser host crystals. A purely first-principles density functional theory-configuration interaction (DFT-CI) hybrid computational method has been developed to accurately compute multiplet energy levels for single atoms of carbon, nitrogen, oxygen, sodium, aluminum, silicon, titanium, and chromium. The multiplet energy levels have been computed with close experimental agreement in terms of magnitude and degeneracy, and the method does not depend on empirical information (i.e. parameters). The computed multiplet energy level results are distributed according to term symbols, which are then compared to experimentally-observed multiplet energy levels. The hybrid method consists of analytic computation of two-electron integrals via the DFT-based orthogonalized linear combination of atomic orbitals (OLCAO) method, which are subsequently used as input for the CI-based discrete variational multi-electron (DVME) method to obtain the multiplet energy values.

**Keywords:** exchange-correlation; electron repulsion integral; multiplet; DVME; OLCAO; density functional theory; configuration interaction















## ABS-2 Soil decontamination by cesium-free mineralization with CaCl2: effect of chlorine on phase transformation of a clay mineral

Iwao Shimoyama

Japan Atomic Energy Agency

As shown in the cases of nuclear accidents in Fukushima, a key issue of environmental remediation is management of contaminated soil. Soil decontamination is generally difficult because radiocesium is strongly fixed in micaseous clay minerals in soil. Cesium-free mineralization (CFM) has been proposed as a new soid decontamination method. While conventional heat treatments utilize physical melting of soil above 1000°C, CFM ulitizes chemical reaction of clay minerals at lower temperatures and can convert clay minerals to other minerals which adapt for industrial use. Precident works imply a catalytic effect of Cl which facillitates phase transformation of clay minerals, however, the detail of the reaction is not clear. In this work, I used Cssorbed weathered biotite (WB) as a model soil and analyzed chemical bonding states of Cl in WB in the early stage of the reaction before phase transformation using near-edge X-ray absorption fine structure (NEXAFS) spectroscopy. Afrer heat treatments with CaCl2, Cl K-edge NEXAFS spectra of the samples were interpreted based on electronic structures of Cl sites in some model clusters using the DV-X $\alpha$  method indicating that high valent Cl ions which bond with O in the clay mineral were formed in the early stage of the reaction. Furthermore, we calculated total energy of model clusters, which mimics siloxane-ditrigonal cavity of micaceous clay minerals. Discussion on structural stability indicates that Cl in the reagent can destabilize the silica network by bonding with O in clay minerals and consequently plays a role to decrease reaction temperature for phase transformation.















# ABS-3 Sorption characteristics of ferrocyanide nanoparticles to metal ions in nitric acid solution for development of vitrification processes of high level radioactive nuclear wastes

J. Onoe, S. Watanabe, M. Harigai, Y. Inaba, and K. Takeshita

Nagoya University, Tokyo Institute of Technology

High-level radioactive nuclear liquid wastes (HLLW: radioactive metal ions in 2 M nitric acid solution) are generated in the reprocessing of spent nuclear fuels or in the decommissioning of nuclear reactors. In the process of producing the vitrified objects containing the wastes by using a glass melter, platinum-group metals (PGMs) [especially, ruthenium (Ru), rhodium (Rh), and palladium (Pd)] and molybdenum (Mo) cause serious problems: PGMs tend to be accumulated on the sidewall surface of the melter, whereas Mo compounds, so called yellow phase, are formed in the vitrified object. These issues result in (i) degradation of vitrified objects due to heterogenization and (ii) an increase in both disposal space and processing costs in conjunction with additional vitrified rods obtained by flushing the glass melter. To solve these issues, we have developed a process for efficient removal of PGMs and Mo from HLLW prior to introducing into the glass melter, using metal hexacyanoferrates (HCF) as a sorbent [1-3]. It is important to reveal the sorption mechanisms of PGMs and Mo for design of high performance HCF sorbents. In this talk, we will present the results on the sorption characteristics of Prussian blue (PB) nanoparticles, one of the HCFs, to the above metal ions in nitric acid solution. obtained using various spectroscopies and first-principles calculations.

[1] S. Watanabe et al., J. Appl. Phys. 119, 235102 (2016).















[2] S. Watanabe et al., AIP Adv. 8, 045221 (2018). [3] S. Watanabe et al., Chem. Phys. Lett. 723, 76–81 (2019).

**Keywords:** ferrocyanide nanoparticles, sorption characteristics, nuclear wastes, vitrification processes















### ABS-4 Crystal Size Effect in Polaritonic Luminescence from Atomic Cryocrystals

Alexander Ogurtsov, Olga Bliznjuk, Nataliia Masalitina

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The exciton-photon interaction leads to the formation of polaritonic states energetically positioned at both sides of the initial exciton. In a large ideal crystal of cubic symmetry, where the interval of the longitudinal-transverse splitting does not contain excitonic levels, the polaritonic dispersion branches lie beyond this interval at both sides of its boundaries. On the contrary, in a crystalline grain comparable or less in size than the wavelength in the substance, the interval of the longitudinal-transverse splitting is filled in continuously by excitonic states intercepting a significant part of the oscillator strength of the excitonic transition. The photoluminescence spectra of atomic cryocrystals (solid Xe and Kr) were measured at the Superlumi experimental station at HASYLAB, DESY, Hamburg. Unlike previous works, where the red polaritonic shift was small commensurably with a weak inelastic polaritonphoton scattering, a large polaritonic shift of luminescence is not due to energy dissipation, the energy conservation law being met due to equal probabilities for opposite-sign energy shifts. Such effect is possible if the crystalline grains are comparable in size with light wavelength, which provides the filling in the interval of the longitudinal-transverse splitting by excitons with sufficient oscillator strength. And the sample structure must be perfect enough to lowering the exciton scattering rate with respect to the rate of the polariton formation through exciton-photon coupling. For the first time the excitation spectra of free-exciton luminescence band were recorded simultaneously below the bottom of excitonic band E and within the interval of the longitudinal-transverse splitting. The luminescence of non-equilibrium polaritons was observed















both within the longitudinal-transverse splitting interval and at photoexcitation below E. The excitation spectrum below the bottom of excitonic band is determined by competition of two processes. The first one is the creation of excitons by photons with energy E at the Lorenz tail of excitonic absorption. The second process is a competing absorption related to the direct formation of two-site excitonic polarons (self-trapped excitons). Both excitation spectra of polaritonic luminescence below E and within the longitudinal-transverse splitting interval show high sensitivity to crystal quality of the samples

**Keywords:** exciton-photon interaction, longitudinal-transverse splitting, inelastic polariton-photon scattering















### ABS-5 Supramolecular Rare Sugar

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#### Abstract

We introduce rare sugars including their derivatives and supramolecular rare sugars, that have been actively researched at Kagawa University. Although rare sugars are special sugars which hardly exist in nature, we has succeeded in mass synthesis of rare sugars by utilizing biological enzyme isomerization reaction. In addition, rare sugars have various functions such as blood sugar level suppressing function, cancer cell growth suppressing function, and antibacterial action. In addition, since rare sugars have a large number of hydroxyl groups, they have a possibility for using as devices for expressing various functions by employing them as ligands of transition metal complexes. In recent years, it is successful that we have synthesized the suplamolecular rare sugars (SRSs) from the different types of rare sugars, that is not as simple mixtures but as single crystals having superlattice structure, that can be freely controlled optical rotation. It has been found that the crystal structures of these SRSs mostly follow the Wallach rule, but do not satisfy the Wallach rule especially in the case of D,L-psicose. Therefore, we have investigated the single crystal X-ray structural analyses of SRSs, obtaining the detailed crystal structure data, and analyzed the intermolecular interaction between their sugar molecules in the















crystal by means of the DV-X $\alpha$  molecular orbital calculation. According to our detailed analysis of the research, calculating the intermolecular interaction revealed that the stability of the intermolecular interaction in the crystal can not be explained only by following the simple Wallach rule. Specifically, for example in the case of D,L-psicose, the total energy in a crystal can be stabilized by aligning the polarization vectors of the molecules, and as a result, we have clarified that the SRSs crystal structure can be stabilized, even if it does not follow the simple Wallach rule.

**Keywords:** supramolecule, rare sugar, crystal structure

**Topic:** DV-Xa Method















#### ABS-6 X-ray Absorption Spectroscopy and Its Simulation for Some Metal Oxides

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X-ray absorption spectroscopy (XAS) is an easy and nice method to examine the chemical and local structural properties of materials which measures the X-ray absorption coefficients with various incident X-ray energies. XAS can reveal the atomic coordination and the intersite or intrasite electron-electron interactions for each atomic species, so that it can be commonly employed for identifying the local electronic structures of condensed matter.

In this talk, I would like to overview the general principles of XAS for the local structural identification, and showcase some examples of theoretical considerations for metal oxide systems including manganites, double perovskite cobaltites and hafnia-zirconia. For the simulation of soft XAS spectra, the concept of configuration interactions with atomic multiplets is employed. For the simulation of hard XAS spectra (so-called XANES), the ab-initio real space multiplet scattering calculation (FEFF) is employed.

**Keywords:** X-ray absorption spectroscopy, XANES, FEFF, Configuration interactions, Atomic multiplets















## ABS-7 Study on The Higher-Order Structure and Hydrogen Bonding of Biodegradable Polymer by Low-Frequency Vibrational Spectroscopy

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Synthetic polymers, including plastic products, are known as one of the most important materials in modern life. They have been widely used in various fields such as energy, information technology, medical, living, and environment. However, most of them cannot be decomposed in the environment causing environmental problems and harmful for living organisms. More than that, the excessive use of synthetic polymer will result in the depletion of irreplaceable natural resources since most of them are made from petrochemical materials. Therefore, development of new biopolymers is expected as a material to replace fuel-based polymers. Among them, chitosan is abundant in nature. Development of polymers with chitosan contributed to solve the environmental and resource depletion problems. It is getting more attention as a new material that mitigate energy waste. Chitosan is a polysaccharide produced by deacetylation of chitin and is extensively used in drug delivery applications. Chitosan is difficult to use industrially because it has high glass transition temperature (Tg) and high crystallinity, and exhibits high elastic modulus and low strain fracture. Therefore, it is necessary to improve their physical properties by blending















or copolymerizing with other polymers. Intermolecular hydrogen bonding between chitosan and other polymer molecules is expected to play an important role in stabilizing the higher-order structure. The information related to this interaction can be observed in the low-frequency region (3.3-330 cm-1) using terahertz (THz) and low-frequency Raman spectroscopy. Since lowfrequency vibrational spectra are derived from intermolecular and intramolecular interactions. THz and low-frequency Raman spectroscopies can be powerful tools to reveal the formation of higher order structures of not only homopolymer but also polymer blends. In this study, by analysing this low-frequency vibrational spectra, we attempted to elucidate the change in higherorder structure and intermolecular hydrogen bonding formed by polymer blends of chitosan and other polymers.

**Keywords:** Chitosan, higher-order structure, hydrogen bonding, low-frequency vibrational spectroscopy















## ABS-8 Systematic First-Principles Calculations of Charge Transfer Transitions of Transition Metal Ions (Sc3+, Ti3+, V3+, Cr3+, Mn3+, Fe3+) in α-Al2O3 with Structural Optimization

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The position of the impurity level within the band gap is very important in optical materials. It can be estimated by calculating the charge transfer transition energy from the valence band to the impurity levels (Ligand to Metal Charge Transfer: LMCT). Recently, we successfully reproduced the LMCT energies and their experimental trend of transition metal (TM) ions in  $\alpha$ -Al2O3 using the DVME method considering the configuration-dependent correction and the lattice relaxation based on the Shannons crystal radii. We also clarified that the LMCT energy is very sensitive to the bond length. In this work, in order to calculate the LMCT energies for various trivalent TM ions in α-Al2O3 using more accurate model clusters, we performed structural optimization using the CASTEP code and constructed the optimized TMO69- and TMAl13O630+ clusters (TM = Sc3+, Ti3+, V3+, Cr3+, Mn3+, Fe3+). As a result, the trend from Sc to V was reproduced better by calculations using the optimized clusters. The differences between the LMCT energies of the optimized clusters and those of the relaxed clusters based on the crystal radii originate from the multiplet splitting of the LMCT states.

**Keywords:** Charge transfer transition, Multiplet, Structural optimization















#### INTERNATIONAL CONFERENCE ON DV-Xq METHOD

## ABS-9 Prediction of 4f2→4f15d1 transition energy of Pr3+ in fluorides based on first-principles calculations and machine learning

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The 4f2-4f15d1 transition energies of Pr3+ in fluorides are utilized for various optical materials such as solid-state lasers, phosphors, and scintillators. Therefore, it is important to predict such energies of unknown materials for theoretical design of novel optical materials. In this study, we tried to predict the 4f2-4f15d1 transition energies of Pr3+ in fluorides based on first-principles calculations and machine learning. The first-principles calculations were performed based on the relativistic discrete variational multi-electron (DVME) method using the model clusters composed of the central Pr3+ and the anions closer than the nearest cation. Although the calculated 4f2-4f15d1 transition energies of Pr3+ in fluorides showed a relatively good correlation with the experimental ones, the theoretical values tend to be overestimated by ca. 2 eV. In order to improve the accuracy of the prediction, we used the calculated transition energies as an attribute for machine learning. As a result, the regression formula to predict the 4f2-4f15d1 transition energy of Pr3+ in fluorides has been derived by machine learning using the theoretical 4f2-4f15d1 transition energy as well as some other electronic and structural parameters as the attributes. The accuracy of the prediction was significantly improved compared to the simple firstprinciples calculations

**Keywords:** The 4f2-4f15d1 transition energies of Pr3+ in fluorides, machine learning















### ABS-10 Optimization of first-principles calculation conditions of multiplet energies in Fe3 + and Co3 + in $\alpha$ -Al2O3

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The prediction of multiplet energies of dn ions such as transition metal ions in crystals is important for the development of novel optical materials. The first-principles calculations of the multiplet energies can be performed by the discrete variational multi-electron (DVME) method which is based on the configuration-interaction (CI) approach. Although the mutiplet energies calculated by CI calculations are generally overestimated, the overestimation can be corrected by considering the configuration-dependent correction (CDC) and the correlation correction (CC). For example, the experimental multiplet energies of V3+ and Cr3+ in  $\alpha$ -Al2O3 were well reproduced by first-principles calculations considering CDC-CC. However, for d5 and d6 ions, the conditions of CDC-CC such as the considered transition processes have not been established. In this study, in order to optimize the conditions of CDC-CC, we performed firstprinciples calculations of the multiplet energies of Fe3+ and Co3+ in α-Al2O3 considering CDC-CC based on various transition processes. As a result, we could optimize the conditions of CDC-CC for Fe3+ and Co3+ in  $\alpha$ -Al2O3 and successfully reproduced the experimental multiplet energies. By consideration of CDC-CC, the repulsion between electrons was suppressed and the overestimation of the multiplet splittings was reduced.

**Keywords:** First-principles calculation, Multiplet, Transition metal















### ABS-11 Cultivation of Oreochromis niloticus with an **Environmentally friendly Bioflog System**

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Increasing population growth demands the availability of continuous food. Aquaculture is one of the food production sectors that has the highest growth rate in the world. Facing this opportunity aquaculture is faced with several challenges related to the limited natural resources such as water and land, and aguaculture waste disposal. Furthermore, the application of best aquaculture practices in aquaculture product certification requires an environmentally friendly aquaculture practice. Oreochromis niloticus is a kind of freshwater consumption fish and is now a popular pet fish in freshwater pools in Indonesia. This research aims to increase aquaculture production in Oreochromis niloticus maintenance through an environmentally friendly Bioflog system. This research method was designed in form of Research and Development. The results showed that the operation of ponds using minimal water exchange, the development of dense microbial populations and management of microbial populations through C/N ratio adjustments could control the concentration of inorganic nitrogen in water. Bacteria in ponds form bioflog, producing microbial proteins that make it possible to recycle unused feed proteins, there by minimizing the occurrence of pollution.

**Keywords:** Bioflog, Oreochromis niloticus, Environmentally Friendly















## ABS-12 Prediction of 4f7→4f65d1 transition energies of Eu2+ in oxides based on first-principles calculations and machine learning

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Eu2+ ions are utilized as luminescent ions in solid-state lasers and phosphors. Therefore, the prediction of the 4f7→4f65d1 transition energy of Eu2+ in crystals is important to develop novel luminescent materials. In this work, we tried to predict the 4f7→4f65d1 transition energy of Eu2+ in oxides using first-principles calculations and machine learning. The first-principles calculations were performed based on the discrete variational multi-electron (DVME) method using small clusters composed of Eu2+ and all anions closer than the closest cation. Although the calculated 4f7→4f65d1 transition energies and the experimental ones showed some correlation, the theoretical values tend to be larger than the experimental ones by ca. 1.5 eV. Since machine learning enables one to create a predictive model of an output based on attributes, we tried to create a predictive model of the  $4f7 \rightarrow 4f65d1$ transition energy of Eu2+ in oxides by machine learning using the calculated 4f7→4f65d1 transition energies and other electronic and structural parameters as the attributes. The obtained predictive model significantly improved the correlation between the predicted 4f7→4f65d1 transition energies and the experimental ones.

**Keywords:** Machine larning, Multiplet, 4f-5d transition















### ABS-13 Lattice Relaxation Effects on the Multiplet Energies of Ruby Under Pressure using One-Electron Calculations

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Up to recently, it has been difficult to calculate the multiplet energies of compounds using one-electron approach. Since it only considers one electron and one nuclei, the interaction among the electrons are neglected. Previously we have successfully estimated the 2E and 4T2 levels of ruby at 0 pressure using one-electron approach based on Ohnisi's method. We also compare the result with those calculated by many-electron approach. The one-electron approach carried out in this work is a first-principles Discrete Variational-Xα (DV-Xα) calculation. In this work, we want to perform similar study not only at 0 pressure but up to 110 GPa. We estimated the lattice relaxation effect due to the Cr3+ substitution and due to the applied pressure by using two different methods i.e., Shannon's crystal radii and geometry optimizations. Two different types of model cluster consisting of 7 and 63 atoms will be used. The 4T2 level is simply estimated by the crystal field splitting (10Dq). Whereas the 2E level is estimated by the barycenter of t2g3 configuration.

**Keywords:** pressure, first-principles, CASTEP, a-Al2O3















### ABS-14 Optical properties of Co3+ doped in α-Al2O3 with Considering Lattice Relaxation Effect

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In this work we estimated the optical properties of  $\alpha\text{-Al2O3}\colon Co3+.$  We constructed model clusters consisting of 7 and 63 atoms. The lattice relaxation effects due to the Co3+ substitution were calculated using Shannon's crystal radii method and geometry optimizations in the Cambridge Serial Total Energy Package (CASTEP) method. The one-electron Discrete Variational-X $\alpha$  (DV-X $\alpha$ ) method was used to estimate the molecular orbital energies, while the many-electron Discrete Variational Multielectron (DVME) method was used to estimate the d-d absorption spectra.

Keywords: Co3+, a-Al2O3, first-principles, DV-Xa, DVME















### ABS-15 Effects of Transition Metal Doping to Cerium-Oxides in Thermal Reduction Reaction

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Considering our lives, novel energy production is so required, and many scientists have been investigated this problem from a lot of views. One of the ways for the new energy productions is the solar power thermochemical production by an oxidation-reduction reaction of the ceramics CeO<sub>2</sub> (ceria). In this research, the ceria is used for obtaining an H<sub>2</sub> gas in vapor reaction in high-temperature thermal equipment which has a heat production system consisting by focused sun light. Nowadays technology has been also developed to keep a human living, not to harm the Earth environment. From these points, it is realized that how the H<sub>2</sub> gas is important for our lives, so we are trying to improve the thermochemical H<sub>2</sub> gas production by means of a ceria as a catalyst. Our purpose in this study is, to point out what effects occur in doped ceria's thermal reduction (TR) reaction by using DV-Xα method. Comparing the















models between the pure ceria and the Mn doped ceria, we have realized the difference by the reaction. In this appearance, one of the considerations is a view from p-DOSs (partial-Density of States), in which there are different O-2p DOSs by different crystal structures. From this view, we considered that the ceria structure would become more stable and more flexible to cut the Ce-O bonding to keep the stable cyclic thermal reaction in Mn doped ceria.

**Keywords:** Ceria,  $H_2$  gas, Thermal reduction (TR), Mn doped ceria















### ABS-16 Study of LCAO-MO calculation by using completely numerical basis functions

Katsumi Nakagawa

MO BASICS Research

#### Introduction)

DV-Xa method uses numerical basis functions adaptable for the circumstance in a molecule. But they are calculated based on spherically symmetric potential for each atom. Newly proposed method inherits DV-Xa's merit but isn't restricted by the premise of atomic spherical symmetry. Aim of the study). This method is being developed as a powerful tool to calculate MOs under complicated outer potential, especially vector potential.

#### Method)

Basis functions are calculated by operations of matrices representing physical quantities and vectors representing wave functions. Analytical assists, like spherical harmonic functions, are not necessary at all. Hartree-Fock-Slater equations for molecules can be expressed numerically even for arbitrary outer potential and solved easily as eigenvalue problems of matrix. But basis functions for an atom are defined only on sample points proper to that atom. On the other hand, basis functions need to be defined on all sample points to calculate Fock matrices for LCAO-MO calculation. The author will explain some techniques to pass over this gap at this presentation.

#### Results)

LCAO-MO calculations were tested within real wave functions. Total energy vs interatomic-distance curves for















N2, F2 and CO were calculated and showed minima near experimental equilibrium distances. Dipole moments of CO, O3 and NH3 were calculated and matched semi-quantitatively experimental moments. Calculations of basis functions were heavy but showed O(n) dependence.

#### Conclusion)

It was demonstrated that basis functions calculated by matrix operation can be used well for LACO-MO calculation. When wave functions are extended to complex, this method will serve as a useful tool to treat MOs under complicated magnetic fields.

**Keywords:** DV-Xa method, numerical basis functions, vector potential, dipole moment















### ABS-18 Controlling of the Spin State by Jahn-Teller Distortion in Octahedral Hexa- Coordinate Metal Complex

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Metal complexes exhibit significant physical properties such as electrical conductivity, magnetism and optical properties. They can be controlled by changing the ligand field splitting of the d-orbital of the central metal ion. We have investigated the reversible spin crossover phenomenon by changing the ligand field splitting in six-coordinated metal complexes ML6. In this study, we focused on the change of the spin states by JahnTeller distortion in the case of an octahedral hexa-coordinated metal complexes ML6, involving 2 types of different ligand molecules. In addition, we have used DV-X $\alpha$  and DVME methods in order to calculate the electronic state. In order to reproduce the effect of the JahnTeller distortion in the calculation, a uniaxial anisotropic distortion has been applied into the octahedral hexa-coordinate metal complex. The purpose of this research is to study the mechanism and phenomenon of the spin state changing by studying the spin crossover phenomenon.

**Keywords:** Complex















### ABS-19 Single-Crystal X-Ray Structural Analysis and Electronic Structures Calculation of Rare Sugar

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There are two types of mono-saccharide sugars in nature, which are natural monosaccharide and rare sugar. The sugar that exists in extreme few amount in nature is called as rare sugar e.g. D-psicose, D-allose. The reasons we choose the rare sugar as a research target are because the rare sugar has almost no calories and is very useful for diabetic and dieter patients. Specifically, D-psicose is a no-calorie rare sugar with the sweetness of about 70 % of a sucrose. It has been confirmed that taking the D-psicose with meals suppresses the rise of sugar into the blood. Further, it is very effective in improving and preventing the diabetes. In order to investigate a research on the rare sugars, the first step must be to obtain the correct molecular structure. However, few crystal structures of rare sugars have been reported up to now. Therefore, the purpose of this research is to analyze the singlecrystal X-ray structure of unknown rare sugar 'L-glucose'. In addition , the DV-Xamolecular orbital method is used to compare the differences in a hydrogen bonding between Dglucose and L-glucose, and to make a novel supramolecular rare sugar.

**Keywords:** Rare Sugar, D-psicose, L-glucose, Supramolecule, Hydrogen bonding.















### ABS-20 Data Mining Application with Fuzzy Logic Method for Monitoring Vehicle Position Based on Android

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Universitas Islam Sultan Agung

Cases of vehicles theft in the Central Java region occurred 869 cases, the percentage was 57.86% against other crimes. To prevent vehicles theft, the police need public participation by increasing awareness of their vehicles. Vehicle theft can occur due to owner negligence and lack of safety locks on the vehicle. This study aims to create data mining application as monitoring vehicle position. The transmitter WiFi 2.4 GHz placed on a vehicle, then measured the RSSI signal by an android application based on fuzzy logic. Indication of theft is that the vehicle is positioned away from the owner, so the signal RSSI is less than -90 dBm. Fuzzy logic monitors this change in distance. When the membership function is lost, fuzzy logic instruct android to activated the alarm. Fuzzy logic was able to make decision give a alarm to user when RSSI signal less than -90 dBm. RSSI signal is less than -90 dBm when the distance is 20 meters if there is a wall barrier, without obstacle the distance is up to 80 meters. RSSI signal is influenced by the measurement environment.

**Keywords:** Data mining application, Fuzzy Logic, Monitoring vehicle position















### ABS-21 An elaborate response in molecular random network - Approach for information processing functionality-

Megumi Akai-Kasaya

An animate brain consists of interconnected complex biological networks of locally active components. The informational processing exploits massive parallelism with low energy consumption, utilizing the multiplicity and stochasticity of signals. Recently, utilization of desiglees random networks of inanimate matter for computation or informational processing has started to be proposed. Here we introduce two nanomaterial networks, which show complex response showing potency for advanced future signal processing.

We succeeded in showing experimental evidence to prove Coulomb blockade taking place on Two-dimensional organic conducting polymer films. Electrical conductivity of hexylthiophene monolayer showed temperaturedependent threshold voltage in temperature range of 150K—4K and increased in power law of the current-voltage beyond the threshold. The onset of two-dimensional Coulomb blockade in the organic thin film was theoretically verified through the calculation of the delocalization of electric charge in the molecular film. This system meets the criteria to be a suitable building block for the physical realization of a cellular neural network. We further found a neuromorphic device that consist of extremely dense and random single-walled carbon nanotube (SWNT) complexed with polyoxometalate molecule generating spontaneous spikes similar to nerve impulses of neurons. A simulation calculation of the random molecular network model, which are able to store electric charges, replicate spikes generated from the network. This molecular model would very likely become a component of reservoir computing that is















anticipated as next-generation artificial intelligence. These results indicate the possibility that complex functional networks can be constructed using molecular devices, and contribute to the development of neuromorphic devices.

**Keywords:** Nanomaterial Molecular Device Neuromorphic Neural Network















### ABS-22 Prediction of emission energy of Cr3+ in oxides based on first-principles calculations and machine learning

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Kwansei Gakuin University

Transition-metal ions with d3 electronic configuration such as Cr3+ and Mn4+ are utilized as emission centers in various luminescent materials such as ruby (Cr3+-doped  $\alpha$ -Al2O3) or alexandrite (Cr3+-doped chrysoberyl). Since it is difficult to investigate the multiplet energy levels of Cr3+ in a wide variety of oxide crystals experimentally, the theoretical prediction of the energy of the emission level (2Eg) is indispensable for the efficient development of novel Cr3+doped luminescent materials. In this study, we predicted the multiplet energy of the emission level (2Eg) of Cr3+ in oxides by first-principles calculations based on the discrete variational multi-electron (DVME) method using relatively small clusters consisting of seven atoms. However, the correlation coefficient between the calculated 2Eg energy and the experimental ones was relatively low (0.52). In order to improve the accuracy of the prediction, we also performed a machine learning modeling. By using the calculated 2Eg energy and the other electronic and structural parameters as the attributes, we created the predictive model of the 2Eg energy of Cr3+ in oxides. The predicted 2Eg energies are in good agreement with the experimental ones, showing a high correlation coefficient of 0.92.

Keywords: Cr, DV-Xa















### ABS-23 Consideration of Super Atomic Hibrid Orbital in Super Atom M@Al12 (M = Be, Mg, Ca, Sr)

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We introduce SuperAtom, which is called a modern alchemy and has been studied around the world. The SuperAtom is a nanocluster composed of multiple atoms, for example Al13. But very interestingly, the "SuperAtom" can mimic the chemical properties of "atom", for example, the Al13 exhibits the halogen atom Cl. If this SuperAtom is constructed to an appropriate size and can be synthesized freely, there is the possibility to be placed as an "artificial atom" in a three-dimensional periodic table such as the conventional two-dimensional periodic table. In recent years, the exhaustion of rare metals has become a big problem, so that in the next generation of materials and devices, the SuperAtoms play as an important role, and it is expected to be used for various materials or as a substitute for expensive metal catalysts such as Pt. From these points of view, the SuperAtoms have been studied all over the world up to now, but there is not much studies on their electronic structures. Therefore, in this study, we have analyzed the electronic state of the chalcogen-inclusive type SuperAtom M@Al12 (M = Be, Mg, Ca, Sr) by means of DV-Xα molecular orbital calculation. Our analysis revealed that the electronic configuration of the SuperAtom, which









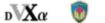






changed only the central atom, depends largely on the kind of doped atom. And we can also confirm the "SuperAtomic hybrid orbital" composed of SuperAtomic orbitals, and chalcogen characteristics.

Keywords: SuperAtom, SuperAtomic Hibrid Orbital















#### ABS-24 Mechanism of Optical Rotation of Amino Acids Using Electronic State Calculation

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Because of the chiral nature of the building blocks of living matter, an optical phenomena associated with the chirality constitute an important topic in physical chemistry. The specific optical rotation, which is a parameter for the characterization of the natural optical activity, depends strongly on the conformation of the molecule. In this study, we investigated the dependence of the optical rotation on a molecular conformation in the gas phase by calculating the electronic states of seven kind of chiral amino acids using the DV-X $\alpha$  method. As a result, we can confirm the existence of an antibonding orbital on the side chain and the optical rotations are strongly related.

**Keywords:** Chiral Optical Rotation















### ABS-25 Generation of Two-Dimensional Spectrochemical Series in Tetrahedral Complexes

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The physical properties of metal complexes that are present in many places are due to the ligand field splitting of the dorbital of the central metal ion, and the series representing the relationship of the ligand field splitting is called a spectrochemical series. This spectrochemical series represents the relationship of the ligand field splitting in the octahedral hexa-coordination structure, but no equivalent index has been shown in the tetrahedral four-coordination complex. In this study, we have investigated the creation of a novel spectrochemical series in tetrahedral fourcoordinated metal complexes. As a result, it is possible to accurately understand the ligand field splitting of the tetrahedral four-coordinated metal complex, and to more effectively apply the energy for obtaining a spin crossover phenomenon in which the magnetic spin state reversibly changes. As a research flow, first, a tetrahedral structural model is created, and then the ligand field splitting is calculated using the DV-Xa method to create spectrochemical series. As a result, we succeeded in creating a spectrochemical series of tetrahedral metal complexes. It has been found that the spectrochemical series of tetrahedral four-coordination complexes tend to hold as they are in octahedral hexa-coordination complexes to some extent, but there are cases where the series does















not hold according to the peculiarity in the case of the four-coordinated metal complex.

**Keywords:** Spectrochemical Series, Four Coordination Complex















### ABS-26 Effect of Molecular Distortion of Ligand Field Splitting in Five-Coordinated Metal Complex

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Metal complex indicates the significant physical properties such as magnetism, electrical conductivity and an optical property due to the electronic interaction between the ligand molecule and the central metal ion. We have evaluated the magnetism of the metal complex by controlling the ligand field splitting, which is the energy splitting of the d-orbitals. The magnetic phenomenon of such compounds are realized as a result of the electronic state based on the transition metal coordination complexes, and which can be switched between high spin (HS) and low spin (LS), that is called a spin-crossover (SCO) phenomenon. Our group have been investigated the way how to control the spin state according to the concept of a distortion. The five-coordinated metal complex ML5 has been experimentally confirmed to be a molecular distortion called the Berry pseudorotation (BPR). In the BPR process, both the axial and equatorial ligands can move at the same rate of increasing the angle between the other axial or equatorial ligands in five-coordinated metal complex. The classical BPR mechanism changes its molecular symmetry between two independent trigonal bipyramidals (TBPs) of D3h symmetry via a square pyramidal (SP) of C4v symmetry. The distortion parameters 5 are proposed in order to represent the distortion of the BPR process quantitatively. In this work, we predicted the possibility of the SCO















phenomenon in intramolecular exchange mechanism through the BPR process in a five-coordinated metal complexes.

**Keywords:** Spin-crossover, Berry pseudorotation, Five-cooridnated Metal complexes















### ABS-27 Single crystal X-ray structural analysis of sugar molecules and electronic theory

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Rare sugar is a monosaccharide that there are trace amounts in nature, natural sugars present in large amounts in nature is referred to as a natural monosaccharide. Recently, the isomerase called D-tagatose-3-epimerase (DTE) was discovered, and it has a possibility to synthesize quantity of the rare sugar from a natural sugar through the enzymatic reaction. And all of hexoses can be synthesized by four kinds of enzymatic reactions (oxidoreductase reaction, aldose isomerase reaction, aldose reductase reaction and DTE reaction). In this study, single-crystal X-ray structure analysis of a sugar alcohol and its derivative have been performed in order to determine the absolute coordinates of these sugar molecules. We give an electronic state calculation by means of the DV-Xα method using the obtained data of the absolute coordinates. We also consider that mechanism of the enzymatic reaction intermolecular energy properly such as a hydrogen bond in order to synthesize the supramolecular rare sugars (SRSs) which can be controlled their structures and the hydrogen bonds.

**Keywords:** supramolecule rare sugar, hydrogen bond, D-tagatose-3-epimerase















## ABS-28 Structural changes in graphene oxide induced by silver nanoparticles – TERS study

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This work has investigated structural changes of graphene oxide (GO) in silver/graphene oxide (AGO) nanocomposites using tip-enhanced Raman scattering (TERS), which is a combination technique of surface-enhanced Raman scattering (SERS) and scanning probe microscopy (SPM). Based on SERS, a Raman spectrum of trace molecules adsorbed on rough metal surfaces/nanoparticles can be collected. On the other hand, nano-scaled topology of samples can be bestowed by SPM. As a result, TERS provides benefits of those two techniques, enabling one to determine molecular information of diminutive samples at specific nano-scaled areas. Because of this markedly high spatial resolution of the TERS technique, the structural changes of GO in AGO can be achieved by constructing lineprofile TERS spectra straight from the center of silver nanoparticles (AgNPs) on GO layers. The results show evidences that AgNPs cause shortening of C-C bonds beneath AgNPs, flattening of GO layers, and critical bending on GO layers. Additionally, a connection of carbon atoms via















C–C network subsequently expands structural changes with the distance of 200–250 nm from the center of AgNPs, even though this distance is larger than the size of AgNPs. The proposed model of GO structural changes opens new understanding about changes in properties from GO to AGO nanocomposites, which will contribute to a development of advanced nanostructures /nanocomposites in the near future.

**Keywords:** Tip-enhanced Raman scattering (TERS), Graphene oxide (GO), Silver nanoparticles (AgNPs), Silver/graphene oxide (AGO) nanocomposites, Structural changes.















### ABS-29 Week Hydrogen Bonding of Polymers Studied by Terahertz and Low-frequency Raman Spectroscopy

Harumi Sato

**Kobe University** 

The absorption peaks observed in the terahertz (THz) region reflect a higher-order structure, crystalline structure, and intermolecular interactions such as hydrogen bonding. Therefore, THz spectroscopy and low frequency Raman spectroscopy are unique techniques for analysing higher-order conformations and intermolecular interactions in semicrystalline polymers. We have investigated changes of the higer-order strucure and hydrogen bondins of several kinds of polymers such as poly(glycolic acid) (PGA), poly-(R)-3-hydroxybutyrate (PHB), polylactic acid (PLA), poly(ɛ-caprolactone) (PCL), poly (butylene succinate) (PBS), poly (ethylene terephthalate) (PET) and poly (butylene terephthalate) (PBT), and so on by THz spectroscopy and THz Raman spectroscopy with quantum chemical calculations (QCCs).

**Keywords:** terahertz spectroscopy, low frequency Raman spectroscopy, polymer















### ABS-30 Metal complexes with sulfur-containing ligands

Masahiro Mikuriya and Makoto Handa

Kwansei Gakuin University and Shimane University

Organic chelate ligands are useful to develop metal-organic systems. Especially N,N,S-tridentate thiolic ligands have a great affinity for many kinds of metal ions to form various metal complexes from mononuclear to polynuclear species. On the other hand, the corresponding N.N.O-tridentate alcholic ligands form dinuclear Cull species exclusively. We focused on these systems in the hope of obtaining new feature of metal thiolates, elucidating interesting crystal structures and spectral properties, although most thiolato complexes are diamagnetic. We obtained mononuclear and trinuclear Colli species with 2-[(3 aminopropyl) aminolethanethiol. The Colli species reacted with oxygen to form the corresponding sulfinato Colll species. Their conversion was monitored by UV-vis spectra and DFT calculations were performed for the thiolate and sulfinato complexes. We also obtained molybdenum complexes. We will discuss these features based on the crystal structures.

**Keywords:** metal complexes, thiolic ligand, cobalt complexes, molybdenum complexes















## ABS-31 Contribution of edge-carbon atoms and non-benzenoid rings in graphitic carbons to $\pi^*$ peak profiles in CK-XANES

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University of Hyogo

To analyze the local structure of non-benzenoid rings in graphitic carbons by soft X-ray absorption spectroscopy, CK-XANES of aromatic compounds having pentagonal or heptagonal rings were theoretically analyzed by the first principle calculations. Edge-carbon atoms split the  $\pi^*$  peak into two peaks in CK-XANES. Pentagonal rings in polycyclic aromatic hydrocarbon structure disturb delocalization of  $\pi$  electrons in hexagonal rings. Hence, pentagonal rings split the  $\pi^*$  peak into two peaks in CK-XANES. It is also confirmed that heptagonal rings play a role of a hole in hexagonal carbon layer, and the heptagonal carbon atoms can be regarded as edge carbon atoms. Hence heptagonal rings also split the  $\pi^*$  peak into two peaks. Consequently, edge-carbon atoms and non-benzenoid rings make the  $\pi^*$  peak wider than hexagonal rings.

**Keywords:** Soft X-ray, XANES















## ABS-33 Smart Aquaponics Design Using Internet of Things Technology

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Smart Aquaponic is a system of planting plants and maintaining fish in one container with integrated Internet of Things technology. Aquaponic is the process by which plants utilize nutrients derived from fish feces which, if left in the pond, will become toxic to the fish. Plants function as a filter of vegetation which will break down these toxic substances into substances that are not harmful to fish. Plants also supply oxygen to the water used to maintain fish. With this cycle there will be a mutually beneficial cycle between plants and fish. This system is very profitable, because the land used will not be too large. The purpose of this study was to develop a smart aquaponic system using Internet of Things technology. In this system aquaponics are equipped with sensors that function as monitors and actuators. Actuators can be controlled by users using smart phones. Sensor monitoring can be observed by users using smart phones. The method used in this study uses the Microsoft Solution Framework (MSF) with the waterfall system development method and Object Oriented Development (OOD) method. Stages in this study includes problem identification, preliminary planning and design, piloting and implementation. Conclusion: This smart aquaponics design is ready to be implemented in small scale trials.

**Keywords:** Aquaponic, Internet of Things, Smart Aquaponic System















#### INTERNATIONAL CONFERENCE ON DV-X METHOD

### ABS-34 Stability of carbon-vacancy complexes in $\alpha$ -Fe

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[Introduction & aim of the study] Recent experimental and theoretical studies suggest that the carbon-vacancy complexes are formed in Fe-C alloys. In this work, we have performed first-principles calculations to evaluate the stability carbon-vacancy complexes in  $\alpha$ -Fe. For comparison, nitrogen-vacancy complexes have been investigated. [Method] We employed VASP code to obtain formation energies and stable structures of interstitial solutes Xn (X = C and N, n = 1 to 6) and vacancy (V) complexes. The chemical bonding was analyzed using DV-X $\alpha$  molecular orbital calculations.

[Results & conclusion] The formation energies of carbon-vacancy complexes have been calculated with reference to the total energy of an isolated interstitial atom and an isolated mono vacancy. In the case of carbon-vacancy complexes, the C2-V complex is most stable due to the energy gain by forming the C-C bonding. On the one hand, the N2-V complex is less stable than the N1-V complex. This is due to the repulsive interaction between N atoms. The overlap population analysis reveals that the C 2s – C 2s antibinding interaction is reduced by the C 2s – C 2p bonding interaction. The interaction between the N 2s and N 2p orbitals is not strong enough to cancel the N 2s – N 2s antibonding interaction.

**Keywords:** Steel; defect; solute; interstitial; first-principles















## ABS-35 Recent applications of discrete variational multi-electron method

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The discrete variational multi-electron (DVME) program is a first-principles many-electron calculation program especially designed to calculate multiplet states of transition-metal ions and rare-earth ions in crystals. It is a configuration interaction calculation program based on the discrete-variational Xa cluster method. It has been applied to analyze various optical materials such as ruby, alexandrite, Mn4+-doped fluorides and RE-doped YLF. The variety of multiplet spectra such as d-d, f-f, f-d spectra, and X-ray absorption near-edge structures have been reproduced without any empirical parameters and the origins of the peaks in the spectra have been clarified based on the configuration analysis of the many-electron wave functions. The DVME method have been also utilized to create various energy-structure maps for Mn4+ and Ce3+ in oxides which can be used for theoretical design of novel red phosphor materials for white LEDs. Since systematic first-principles calculations are quite time consuming, we have also begun to create simple predictive models based on machine learning by using the results of the first-principles calculations as the training data. This could accelerate the creation of detailed energy-structure maps. In this presentation, I will show some of the recent applications and future perspective of the DVME method.

**Keywords:** First-principles calculation, multiplet, phosphor, machine learning















## ABS-36 Alternative Solutions For Determining Village Funds Using Weight Product Method

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A country is said to be progressing, if all regions of the country prosper. In Indonesia, the smallest area that runs the government function is the village. The legal basis regarding the village government itself is stated in Law No. 6 of 2014 Republic of Indonesia. In carrying out its functions as a government, the village is supported by village funds. Village funds sourced from the state budget are intended for the development and improvement of the welfare of rural communities. Village funds can go down based on the proposal submitted. The proposal for submitting village funds is processed by a work team called Tim 11. So far, the determination of village funds is still manual and less transparent. Therefore we need a system that can overcome the problem of determining village funds. This research provides alternative solutions regarding the determination of recipients of village funds using the weight product method. There are four criteria in this research, namely the number of residents in an RT area, the standard of living of an RT area, the extent of the area, the level of geographical damage in an RT area. And the object of the research chosen was Kasihan sub-district, Tamantirto village. the results obtained are a priority submission in writing the proposal submitted.

**Keywords:** Decision Support System; Village Funds; Weight Product















# ABS-37 DESIGN OF ELECTRICITY ENERGY SOURCES IN SEMARANG PGRI UNIVERSITY USING OFF-GRID SOLAR PANEL SYSTEMS

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The source of electricity in each university building in PGRI Semarang is obtained from each distribution transformer or power transformer. The power transformer used to distribute electricity in the central building (GP) has a capacity of 400 KVA, while the power transformer used in the main building (GU) has a capacity of 160 KVA. In the previous study, identification of the quality of electrical power in the PGRI University Semarang building, obtained a low power data factor and a large electrical network harmonics. The problem was solved by designing and installing bank capacitors and harmonic filters. To avoid dependence on PLN electricity and not using a generator when PLN electricity goes out, the source of electrical energy is designed by using solar energy sources through Photovoltaic. Solar Panel as an important component of solar power plants, converts sunlight into electricity. Generally we calculate the maximum amount of sunlight that is converted into electricity throughout the day is 5















hours. Electricity in the morning is stored in the battery, so electricity can be used at night, where without sunlight. Based on the identification of the load in the GP is 26.12 KW, then in the design using solar energy as many as 27 solar panels are needed. As for the storage system uses 44 batteries 100Ah battery. Off-grid solar panel systems are only used when PLN electricity goes out or can be used at night. The research method used is observing the amount of electrical load, calculating the capacity of solar panels and batteries, and simulating the model using a Power Simulator.

**Keywords:** Solar Panel, Battery, PLTS off-grid, Charger Controller















## ABS-38 Novel shape analysis method for single bioparticles in aqueous solutions

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Rapid structural analysis methods for biomolecules and biomaterials consisting of single or several molecules in solution represent innovative technologies to reveal their functions because the functions strongly depend on their own structures. However, there presently exist no rapid structural analysis methods for single nanomaterials suspended in liquid environment. Nanopore sensors have been widely used to investigate the volume of particles and molecules passing through the pore by probing temporal changes in the ionic current pulses. These pulse sensors have been developed for not only size but also shape of analyte during recent years. Smaller aspect ratio defined as the ratio of the depth to the diameter and a high-speed current detection system provide greater spatial resolution, i.e. tomograms of a material passing through a nanopore. Here we will report the development of low-aspect-ratio nanopores with a spatial resolution of ca.35.5 nm and the 10 MHz-current-amplifier, resulting in realization of ultrafast time resolutions of 1.0 us for the tomography analysis of a material passing through a nanopore. Combining state-of-the-art technologies with multiphysics simulation methods to translate ionic current data into tomograms of nanomaterials passing through a nanopore, we have achieved rapid structural analysis of single and dabble polystyrene (Pst) beads, and bionanomaterials such















as E-colis in aqueous solutions [1]. In addition, we will also report plasmonic nanopore devices, which enable us to detect Surface-enhanced Raman Spectrum of a material inside a nanopore. The nanopore devices will be innovative technologies for the fields of nanobiodevices and structural biology. [1] S. Ryuzaki, et al., Nanotechnology 28 (2017) 15550

Keywords: nanopore















### ABS-39 Design of Product Monitoring System using Internet of Things Technology for Smart Manufacturing

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The application system in the industrial era 4.0 is currently growing rapidly. One of them is the implementation of smart manufacturing in the industrial sector. In smart manufacturing, production processes can be monitored automatically and real time, starting from material selection, then the production process to the planned product. In this study discussed the design of a monitoring system on smart manufacturing based on internet of things technology. Smart technology is implemented on material scans automatically based on color sensors, then from the material it will also be known that with these materials produce certain products and require any material. In addition, the system will also automatically detect through the initial material to find out which processes will be passed. The methods used include literature studies, system requirements analysis, system design and system testing. The results of this study are in the form of a hardware system design and display of production process monitoring system applications. In the system that is made also a notification is displayed if a bottle neck occurs in the production process

**Keywords:** product, desgin; monitoring; smart manufacturing; internet of thing















### ABS-40 A Novel and Fast Memory Perturbation Method to Increase Exploration in Particle Swarm Optimization Algorithm

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Particle Swarm Optimization (PSO), one of the versatile nature-inspired optimization algorithm, continue to suffer from premature convergence regardless of the rigorous amount of research. Many research had tried to address this issue but often use a complex algorithm which tax on computational time and complexity. This research introduced a novel perturbation method to mitigate premature convergence / to increase exploration while keeping the computational cost at a minimum. The particles memories (i.e the position of personal and global best) are modified by a random multiplier which in turn will 'perturb' the particles' velocity. The implementation of this novel perturbation method in early iterations had resulted in 100% success rate in finding global optima in our benchmark tests (Sphere, Schwefel 2.22, Rosenbrock, Rastrigin, and Ackley problem) - whereas the original PSO failed in all benchmark tests - without adding a significant amount of computational complexity and time.

**Keywords:** PSO, premature convergence, perturbation, exploration















## ABS-41 BIOCONVERSION ON WASTEWATER OF SOYBEAN USING MICROBIAL FUEL CELL

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Microbial fuel cell (MFC) is a technology developed to obtain new sources of renewable energy to produce electricity. It can be an alternative for wastewater treatment and bioenergy producers of renewable electricity. This method requires bacteria to convert substrate in wastewater into electrical energy. The mechanism of MFC were oxidation of substrate by bacteria to produce electrons and protons at the anode. The proton in anode chamber passes through a membrane exchange to the cathode chamber, however the electrons couldn't through. It caused accumulation of electron in anode chamber and then both of electrode had a potential difference, so electron in anode chamber passed through membrane exchange to cathode chamber. In this study used dual-chambers reactors with each compartment having 8 cm × 10 cm × 10 cm of dimensions and 5 mm of thickness. This study was subjected to evaluate the performance of MFC sovbean in wastewatertreatment with bacteria of EM4 to analyze the potentials production of electricity energy. The focus of this study was to evaluate the effect of time to electricity. MFC system was observed for 40 hours, measurement of voltages and electric currents performed every 2 hours. The results showed that there was potential of electricity production from soybean wastewater treatment by MFC. The maximum electricity reached in soybean wastewater















media were voltage 441 mV (at 24 h), the electric currents 170  $\mu$ A and the power density 51, 35 mW/m2(at 24 h after acclimatization). Increasing of time effect to decreasing of electricity produced.

**Keywords:** bioenergy, electricity, microbial fuel cell, membrane, wastewater soybean















## ABS-42 Microscopic crystal field effects in impurity centers formed by the transition metal ions

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First-principles methods of calculations of electronic and optical properties of impurity ions in solids allow for a quantitative treatment of microscopic crystal field effects. In other words, they give a possibility of calculating the impurity ions energy levels for different geometric configurations of impurity centers, including changing chemical bond lengths and angles between those chemical bonds. From these calculations, it is possible to extract the distance dependence of the crystal field strength 10Dq, estimate the electron-vibrational interaction constants, Jahn-Teller stabilization energy, Huang-Rhys factors, Stokes shift between the absorption and emission spectra. The obtained results can be used not only for explanation of the already existing experimental results, but for the prediction of optical properties of new materials. In this presentation several examples of such calculations will be given in detail [1-6] along with discussion of practical importance of the obtained results and their potential predictive power.

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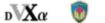






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Keywords: first-principles calculations; crystal field splitting; transition metal ions; Stokes shift















#### INTERNATIONAL CONFERENCE ON DV-X METHOD

# ABS-43 Internet of Things (IOT) with Cloud Computing and Machine to Machine (M2M) communication in Aquaponics Farming Systems

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The IoT is gaining increasing attention. The overall aim is to interconnect the physical with the digital world. Therefore, the physical world is measured by sensors and translated into processible data, and data has to be translated into commands to be executed by actuators. Three important factors propelling the IoT forward are sensing nodes, embedded processing, and communication. This transformation is acompanied with the emergence of cloud computing capabilities supported by an increase in storage capacity, high processing, and Machine to Machine communication for data transport with security. With cloud computing technology, data will be stored and accessed anywhere needed with a support of powerful computing efficient infrastructure performance. storage heterogeneous systems and software which configures and controls these different devices. The Machine to Machine (M2M) communication technology is needed, because the massive explosion of online services, further inspired by the smartphone and handheld revolution, which made these services highly accessible, has created a demand to leverage technology. In this paper, a brief introduction aguaponics farming system is given and the IoT with cloud storage and M2M communication is explained. This will also benefit the IoT in its ease of use in day-to-day life and believe to be future in this area which is getting ready for its revolution.

**Keywords:** Aquaponics, Internet of Things, Cloud Computing, Machine to Machine communication.















# ABS-44 Potential of Ketapang Seed Oil (Terminalia catappa Linn) as Basic Material Mono-diglyceride Biodegradable Surfactant

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Surfactants are widely used in pharmaceuticals, perfumes, cosmetics, food and beverages. One type of surfactant produced from the synthesis of palm oil is mono-diglyceride which can function as an emulsifier. Ketapang (Terminalia catappa Linn) is a beach tree with a wide spread area, whose seeds have not been utilized optimally. The content of Ketapang seed oil has the potential to be converted into mono-diglyceride surfactant. This study uses experimental laboratory methods, while parameter optimization is done by the two level factorial design method. The raw materials used were Ketapang seeds from around the campus of Semarang 17 Agustus 1945 University, n-butanol solvents, glycerol, MgO catalysts. During the glycerolysis process, 8 run experiments were carried out with 3 variables which changed in temperature (60 & 900C); MgO catalyst (2 & 4%) and solvent / 10 g oil volume 20 and 40 ml, while the variable is the weight of 25 gram ketapang seed oil; stirring speed of 400 rpm; reaction time of 4 hours; ratio of glycerol 2.5 ml / 10 g oil; and 24-hour deposition time. From the results of the study, the influential variable is temperature. The optimum results were obtained at conditions of 900C, 4% MgO catalyst, solvent volume of 20 ml / 10g ketapang seed oil and vield 18.27 %. The resulting surfactant has the characteristics of acid number 57.2 mg KOH / gr, saponification number 218 mg KOH / gr.















Surfactant has HLB value 14.75, meaning that the surfactant functions as an O / W type emulsifier or as detergent agent.

Keywords: ketapang seed oil, glycerolysis, surfactant















### ABS-45 BIOPLASTIC FROM JACKFRUIT SEEDS AND RICE WASTE

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This tried to explore characterization studv biodegradable plastic from jackfruit seeds and rice waste. Jackfruit seeds and rice waste contain starch, so it can be used for plastic material with addition of several additives such as polyvinyl alcohol (PVA), glycerol, chitosan and sorbitol. Starch is one of polysaccharides that be used as raw material for biofilms. Polyvinyl alcohol is the most important plastic in making water-soluble films. It was ability to form films, emulsifiers, and its adhesive properties. Polyvinyl alcohol has high tensile strength, good flexibility, and good oxygen barrier. Sorbitol and glycerol are also an additive in the manufacture of biodegradable plastics from starch, which is a plasticizer that increase elasticity. Chitosan have effects to bioplastic, such as biodegradable, hydrophilicity, and anti bacterial. This research aims to determine the effect of addition of PVA, glycerol, chitosan and sorbitol to optimum characteristics of bioplastic. The parameters to be examined bioplastic include thickness, moisture content, tensile strength, and % elongation. Increasing of glycerol added to the plastic material effect to decrease of tensile strength of bioplastic and elongation, lower water resistance and more easily degraded. Increasing of chitosan added to the plastic material effect to higher tensile strength, lower elongation, higher resistance to water and lower degradation. Increasing of PVA added to the plastic material effect to increasing of the tensile strength of the bioplastic and decreasing of elongation of bioplastic, but the increasing of















sorbitol effect to decreasing of tensile strength and increasing of elongation of bioplastic.

**Keywords:** biodegradable plastic, elongation, jackfruit, starch, tensile strength, waste of rice.















## ABS-46 Carotenoid Dynamics Free and Bound to Pigment Protein Complexes: The Role of the 11Bu- State

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### Introduction

The study focuses on the light-harvesting function of carotenoids. How carotenoids capture the photon energy and efficiently transfer its singlet energy to the neighboring bacteriochlorophyll in the pigment-protein antenna complexes (LH2) has been studied. The 11Bu- state in the light-harvesting function are critically investigated, tracing the excited-state dynamics of carotenoids free in solution and bound to the LH2.

### Aim of the study

The goal of this study is to reveal the detailed mechanisms of light-harvesting function. The research focuses on the roles of the 11Bu- state in the light-harvesting function of Cars. A series of investigations were carried out to critically examine the roles of the 11Bu- state in the light-harvesting function.

### Method

The internal conversion processes in Cars were investigated by the use of subpicosecond time-resolved absorption spectroscopy for a series of Cars in solution and bound to the pigment-protein antenna complexes. including neurosporene (n = 9), spheroidene (n = 10), lycopene (n = 11), anhydrorhodovibrin (n = 12) and spirilloxanthin (n = 13).















The SVD and global fitting were applied to of spectral-data matrices.

### Results

The results lead to a branched relaxation scheme of energy deactivation including (1) the singlet internal conversion in the sequence of 11Bu- 11Bu- > 21Ag- > 11Ag- (ground), and (2) the singlet-to-triplet conversion of 11Bu- > 13Ag followed by triplet internal conversion of 13Ag > 13Bu. The relaxation scheme took place in subpicosecond to decapicosecond time scales.

#### Conclusion

The 11Bu- state plays essential roles in light-harvesting mechanisms as a mediator state in the process of internal conversion, an acceptor state in the Car-to-BChl singletenergy transfer and a precursor state for the rapid formation of the Car triplet state.

**Keywords:** Carotenoid singlet energy, relaxation scheme, SVD, Light-harvesting















### ABS-47 Detecting Hoaxes in Indonesian News Using TF-IDF and K Nearest Neighbor

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Universitas Stikubank, Satya Wacana Christian University

The presence of the internet and the rapid growth of social media had given rise to the blossoming of hoax creation and distribution through it. A hoax can cause anxiety and reactivity to its readers and could harm a certain party. Thereby, it is important to detect and report hoaxes to stop its spreading as soon as possible. This research aims to utilize the K Nearest Neighbor (KNN) classification algorithm to detect whether a piece of news is a hoax or not. Experiments were done by using 74 hoaxes compiled from Indonesian hoax-debunking community websites and were being compared against 74 real news from various reputable news websites in Indonesia. The result showed that the model could give detection/classification accuracy up to 83.6% and that the model is prone to false positives detections. The characteristics of the resulted model and further research directions are then discussed

**Keywords:** hoax, fake news, TF-IDF, K Nearest Neighbor, KNN















## ABS-48 **Designing Enterprise Architecture in Koperasi Karyawan** using TOGAF Architecture Development Method

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The Open Group suggests that Enterprise Architecture (EA) can produce an IT blueprint that can be used to determine business, technology and information to support the achievement of the vision and mission of an organization. EA can also be seen as a model, a set of principles and methods used to produce an actual enterprise organizational structure with business processes used covering business operations, business planning, information technology and information systems. EA is also in the form of models, graphs and narratives that will explain the scope of business processes and designs of an enterprise. The purpose of this study is to design EA, especially in Koperasi Karyawan TEKAD Semarang using TOGAF framework. In other words, this architecture is created by emphasizing the relationship between IT and business. EA model is intended to maximize business alignment with IT in all situations, but depends on the nature of business and capacity in business and IT management in cooperatives.

**Keywords:** Enterprise Architecture, TOGAF, Koperasi















## ABS-49 **DECISION SUPPORT SYSTEM MUSEUM AMBASSADOR**USING TOPSIS METHOD

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Faculty of Engineering and Informatics Universitas PGRI Semarang

Generally, the museum ambassador is based on various criteria from several assessment stages. The evaluation criteria for the audition stage are: interview. communication, appearance. Criteria for evaluating the quarantine stage are: creativity, ability, activity, loyalty, responsibility, and written test. Final stage assessment criteria: ideas, communication, and appearance. In the selection process, the committee uses the manual method so it is prone to errors. From these problems to the process of selecting the museum for ambassadors. The decision support system is using Topsis method. SDLC (System Development Life Cycle) is used as a design method. Research shows a score of 100 which means that the system is accepted by the user. While in testing the user test obtained from four respondents got a percentage of 89.24% which means that the system is worth of use. The system is developed in the web. So that is need more research to be developed in mobile.

Keywords: dss, museum, topsis















## ABS-50 Design of Augmented Reality Game app "IntroME" using ADDIE Model

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An understanding of animal classification based on the type of food, is one of the sub themes in the subject of Natural Sciences. In school learning activities an understanding of the classification is conveyed through cooperative approaches such as presentations, group activities and tests. By doing the delivery method it is less attractive for students to pay attention and study in school, as well as to understand it themselves outside of teaching activities by reading books, can reduce students interest in learning it. With the existence of a different alternative in the form of an educational game, it can help in supporting the process of understanding animal classification based on the type of food carried out during teaching activities and outside of school hours. Coupled with the application of augmented reality technology on learning features that can increase user interest in learning, and for the application of learning in the form of interactive games. This educational game uses the ADDIE model and uses the design of the Unified Modeling Language (UML) which consists of Use Case Diagrams, Activity Diagrams, Squares Diagrams and as a programming language in making the application is expected to help solve existing problems. Furthermore, this application will be tested using the Black Box and User Acceptance Test. Based on the results of testing using the















User Acceptance Test obtained a percentage of 86%. Then the test results using Black Box Testing obtained a 100% valid percentage.

**Keywords:** Educational Game; Augmented Reality; Android; ADDIE















## ABS-51 Phosphorus recovery through crystallization of struvite (MgNH4PO4.6H2O): From basic research to applications

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Phosphorus (P) is the eleventh most abundant element on Earth and is essential for life, but its presence in surplus quantities is problematic. Excessive P is responsible for eutrophication of water bodies which causes deterioration of aquatic environments, naturally and economically. Also, excess of P instigates operational problems for industrial facilities due to scale formation and accumulation, which may considerably hamper heat and mass transfer and translates into substantial financial loss. In many cases, the major component of the scale is a phosphate mineral (MgNH4PO4.6H2O), widely known as struvite. In contrast, due to its low solubility and its P content, struvite is an excellent fertilizer. The primary source of P is the phosphate rock, a non-renewable resource, of which about 80% is used as raw material for fertilizers. In line with increasing global population, demand for fertilizers increases rapidly, resulting in the dwindling availability of P world-wide. Thus serious attention is paid for P recovery and reuse. This paper focuses on P recovery from wastewater through crystallization of struvite. Firstly, a brief description of the theory of crystallization is presented. Then, basic research on crystallization of struvite is discussed. Finally, the different processes for P recovery as struvite are described.

**Keywords:** crystallization, Phosphorus, struvite















### ABS-52 The Multi-agents System for Job Recommendation

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Abstract. The number of available job portals causes abundant information. Therefore. а system recommendations is needed by job seekers to find jobs that fit their profile. Offering job vacancies on job portals are changing every time because there are always additional job search data and job opening data. Multi-agents system is a technology that can be used to handle information changes. This article proposed a recommendation system is expected to help job seekers to get jobs in accordance with the field of science they have. The system will monitor what work is offered by online job portals. From the results of observations, the job content offered will be used as a reference so that if new content is entered, the agent will automatically provide input to the job Based on the results of the implementation of the recommendation system using a multi-agent system can provide search results that are in accordance with what is inputted by the user based on the profile they have. These search results can recommend jobs that match the job seeker profile.

**Keywords**: multi-agents system, recommender system Categorized in Computer Engineering















## ABS-53 **DESIGNING ANDROID BASED EDUCATION GAME AKSARA**JAWA USING SHUFFLE RANDOM ALGORITHM

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The lack of appropriate supporting media in learning at the age of children makes the young generation now less familiar and still having difficulty learning Javanese script (Aksara Jawa called in indonesia). For this reason, we need appropriate media in the introduction of Javanese script, one of which is through interesting educational games and can provide information about Javanese script. Games are forms of application that can be used as learning media where the process can be done with the concept of learning while playing for children. In this study the algorithm used was the Shuffle Random Algorithm. With this randomization algorithm, it is expected to avoid repetition of the problem so that the learning process can run effectively. Furthermore, this application was tested using the Black Box, White Box and User Acceptance Test. With the Black Box and White Box testing get a percentage of 100% while with the User Acceptance Test this application has an average of 86%, so it can be concluded that this educational game is feasible to be used as a learning medium for Javanese script.

**Keywords**: Javanese script, Educational Game, Randomization, Android, Shuffle Random















# ABS-54 Electronic state of sulfide-based alkali-ion conducting solid-state electrolytes applied to all-solid-state secondary batteries

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All-solid-state batteries are expected as the next generation secondary batteries for their higher energy density, inflammable properties, and so on. In order to develop these batteries, there are several problems to improve. One of them is the lower ionic conductivities of the solid-state electrolyte. In order to improve the ionic conductivity, electronic states of the sulfide-based alkali-ion conducting solid-state electrolyte were calculated by the DV-Xα cluster method. The cluster models were constructed by the coordination number reported by experimental methods and the bond length estimated from the ionic radii of each ion. The movement of the Li ion was simulated by several model clusters with different positions of the moving ion. The relationship between ionic conductivity and the differential total bond overlap population (DBOP) of the moving ion was discussed for the sulfide-based solid-state electrolytes in the several different systems. In any cases, the smaller change of DBOP of the moving cations played an important role for the fast ion movement in the solid-state electrolytes. This bonding state of the moving cations is one















of the characteristics of the electronic state in the sulfidebased solid-state electrolytes.

**Keywords**: all-solid-state battery, solid-state electrolyte, bonding state analysis, DV- $X\alpha$  method















## ABS-55 Geometry and Stability of Small Gold Cluster Ions by **Graph Theory and Hückel Model**

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Structure and stability of the gold cluster ions of which skeleton are synthesized as a complex was analyzed using the Hückel method based on graph theory. Hückel Energy (HE) and Topological Resonance Energy (TRE) were determined for neutral, positive ion, and negative ion clusters, where all the isomers of the gold cluster up to octamer were considered. Since some graphically designed isomers include bonds that can not be realized in threedimensional space, the screening was carried out by a molecular force field calculation with (lammps.sandia.gov/.). Among the isomers thus obtained, both HE and TRE were most stable when the tetramer was Au 4^{2+} with a tetrahedral structure, and with the hexamer, Au 6^{2+} with two tetrahedrons sharing one side. The complexes with these structures have actually been synthesized. On the other hand, there is no reported synthetic example of the most stable cluster of octamer Au8 with TRE and HE.

**Keywords**: Graph Theory, Hückel method, Gold Cluster















# ABS-57 THE EFFECT OF CHLORIDE ACID (HCL) CONCENTRATION AND FERMENTATION ON BIOETHANOL LEVELS FROM BREADFRUIT (Artocarpus Artilis) SUBSTRATE

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#### **ABSTRACT**

At present the public demand for fuel oil (BBM) is increasing inversely proportional to its availability. One of the efforts to reduce peoples dependence on BBM is to utilize alternative vegetable-based energy such as bioethanol. Bioethanol is a fermented product that can be made from a substrate containing carbohydrates. Breadfruit (Artocarpus artilis) is one of the agricultural products that has a fairly high starch content of 89% and is not included as a staple food source in Indonesia. Utilization of breadfruit is still not optimal because breadfruit is only used as a snack or made into flour. This study aims to make bioethanol with breadfruit raw material (Artocarpus artilis). The method of this study consisted of two stages, the first step was hydrolysis of breadfruit flour with a hydrochloric acid (HCL) catalyst. The concentrations of HCL used in this study were 1%, 1.5%, and 2%. The second stage of fermentation using Saccharomyces cerevisiae with 72 hours fermentation time, 120 hours and 168 hours. From the results of the research it was found that the highest levels of bioethanol to the treatment of HCL 2% concentration and fermentation duration of 168 hours was 17.6%.

**Keywords**: bioethanol, breadfruit, HCL concentration















# ABS-58 Interaction Analysis Application of Arduino Industrial Automation Trainer Based on Project to Improve Cognitive Ability and Bodily Kinesthetic Ability

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Abstract: This research aims to determine the interaction/influence of the application of Arduino Industrial Automation trainer based on projects to enhance cognitive abilities and bodily kinesthetic abilities. college student This research is in the form of quantitative descriptive research. The sample used in this study is one class taken using Saturated Sampling techniques. The research class was treated by using a project-based Arduino Industrial Automation trainer. The independent variables in this study are project-based Arduino Industrial Automation trainer, while the dependent variable is cognitive abilities and bodily kinesthetic abilities.. There are 3 kinds of analysis techniques, namely instrument analysis techniques. prerequisite analysis techniques, and hypothesis analysis techniques. The measured research data are cognitive ability data and bodily kinesthetic ability data. The analysis of the hypothesis test of this study used the T-Test with a significance level of 5%. T-Test Criteria are as follows, Ho is













accepted / H1 is rejected if T count is smaller than T table and Ho is rejected / H1 is accepted if T count is greater than T table. From the results of the instrument test, namely the validation test, there are 75% questions stated valid. For the prerequisite test for the normality of cognitive abilities and bodily kinesthetic abilities on the pretest and posttest obtained L count < L table means the sample is normally distributed. For the prerequisite test for homogeneity of cognitive abilities and bodily kinesthetic abilities obtained F count < F table means the sample is homogeneous. The results of the T test for the first dependent variable cognitive ability obtained T count = 24.41 and T table = 1.697, because T count is greater than T table then Ho1 is rejected, meaning that there is an interaction/influence of the implementation of the Arduino Industrial Automation trainer based on projects in improving cognitive abilities. While the results of the T test for the dependent variable bodily kinesthetic ability obtained T count = 18.33 with T table = 1.697, because T count is greater than T table then rejected, it means that there interaction/influence of the application of the Arduino Industrial Automation trainer based on the project in increasing bodily kinesthetic abilities. So that it can be concluded that there is an interaction/influence of the application of the Arduino Industrial Automation trainer based on projects in improving cognitive abilities and bodily kinesthetic abilities.

Keywords: Industrial Automation Trainer, Arduino, Project,















# ABS-59 ANALYSIS OF THE IMPACT NARRATIVE ALGORITHM METHOD, PSEUDOCODE AND FLOWCHART TOWARDS STUDENTS UNDERSTANDING OF THE PROGRAMMING ALGORITHM COURSES

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University PGRI Madiun

The definition of an algorithm is to describe a problem into a sequence of systematic steps in solving problems. Arranging the algorithm in sequence from beginning to end so that it can solve the problem. The results of the implementation of the algorithm are programs. So the purpose of making an algorithm is to facilitate the making of the program. There are 2 types of algorithms, 1) Text (narration and pseudocode), 2) Visual / image (flowchart). Comparison between the two, students understand it which is higher between the text or visual model. This study aims to see how much infuence the value of students understands the algorithm in text or in an image. In conclusion, students are easier to understand the types of algorithms in an image. The test uses the sample T test, with a 5% significance level obtained value = 0.5. This means that the t count is greater than t table of 2.06390

**Keywords**: algorithm, pseudocode, flowchart, t test















## ABS-60 Prediction of the Number Job Seeker Using Backpropagation Neural Network Method

Khoiriya Latifah, Agung Handayanto, Anita Rahayu

Universitas PGRI Semarang

Problem solving techniques for predicting include Aritical Neural Network. This research aims to apply the Backpropagation Neural Network method in predicting the number of job seekers in the city of Semarang. The data used in this study are secondary data, namely job seekers data of Semarang city residents from Semarang City Manpower Office from 2015-2018. In this study the data will be divided into 2 namely 2015 training data and testing data in 2018. Design and testing in this study using matlab software using 2-3-1 network architecture, which is a multilayer network with 2 input layers, 3 hidden layers and 1 output layer.

**Keywords**: Job Seeker, Neural Network, Backpropagation















## ABS-61 Extraction Sentiment Analysis Using naive Bayes Algorithm and Reducing Noise Word applied in Indonesian Language

Aris Tri Jaka Harjanta, Bambang Agus Herlambang

Universitas PGRI Semarang

Sentiment Analysis is now very important and very useful in machine learning technology where a contextual mining of text to identify and extract subjective information in the source, and in helping to understand social sentiment from comments In general, sentiment analysis can be classified into three broad categories namely sentiment positive and negative. One method of machine learning is the Deep Belief Network (DBN). DBN which is included in the Deep Learning method, is by stacking several algorithms with several extraction features that utilize all resources optimally. This research has two points. First, it aims to classify positive, negative, and neutral sentiments for the test data. The following experiments provide a system of sentiment analysis through the naive Bayes algorithm to calculate sentiment and to improve accuracy by reducing noise in words applied in Indonesian language.

**Keywords**: Sentiment Analysis, Machine Learning, Naive Bayes















#### ABS-62 ABSTRACT

The Effect of Decomposer Microorganism Additions on the Natural Hydroponic Technology (Nht) Systems of Pakcoi Growth

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Nowadays there is a tendency of the people, especially the middle class and above, to choose vegetables with high quality and safe for body. Therefore, farmers are required to always innovate in terms of vegetable cultivation, so that the crops can compete and be accepted by the community. This study aims to determine the effect of the addition of probiotic microorganisms on the Natural Hydroponic Technology (NHT) system on the growth of Pakcoi plants. The study was conducted on May to July 2019 in the agricultural land of Ngesrep Balong Village, Limbangan District, Kendal Regency, Central Java. This study uses a completely randomized design (CRD) with one treatment factor, the type of decomposer microorganisms. The research data was taken through several measurement techniques and direct observation of objects. Data were taken three times on the 14th day, 21st day, and 28th day after planting. Data were then analyzed statistically with ANOVA (Analysys of Variance) at 95% confidence level and continued with LSD test. The analysis shows that the addition of decomposer microorganisms to the Natural Hydroponic Technology (NHT) system can increase the growth rate of Pakcoi plants. Decomposer microorganisms with trademarks ST (Sukses Tani) and EM-4 (Effective Microorganism-4) produce the same growth rate.

**Keywords**: hydroponics, microorganisms, decomposers, Pakcoi















## GALA DINNER, 2 September 2019 The 7<sup>th</sup> International Conference on DV-X $\alpha$ Method (ICDM 2019)

## **Grand Candi Hotel, Semarang, INDONESIA**

MC: Dr. Dyah Nugrahani (Universitas PGRI Semarang, Indonesia)

indonesiaj			
Time	Activities		
19:00-19:10	Opening		
19:10-19:20	"Indonesia Raya" Indonesia National Anthem		
19:20-19:25	Report on ICDM 2019		
	Mega Novita, S.Si., M.Si., M.Nat.Sc., Ph.D		
	(Chairperson of ICDM 2019, Universitas PGRI		
	Semarang, Indonesia)		
19:25-19:30	Speech		
	Prof. Yoshiyuki Kowada (Chair of DV-Xα Society,		
	Hyogo University of Teacher Education, Japan)		
19:30-19:40	Welcoming speech		
	Dr. Muhdi, S.H., M.Hum. (Rector of Universitas		
	PGRI Semarang)		
19:40-19:50	Token appreciation for:		
	- Keynote speakers		
	- Invited speakers		
	- Co-host		
19:50-20:45	Dinner		
20:45-21:00	Closing		















## GUIDELINES FOR PRESENTER(S)

## 2-4 September 2019

## The 7<sup>th</sup> International Conference on DV-Xα Method (ICDM 2019)

## **Grand Candi Hotel, Semarang, INDONESIA**

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- 1. ICDM 2019 distinguished the types of the speaker *i.e.*, keynote speaker, invited speaker, and general speaker
- 2. Keynote speaker(s) has in total 40 minutes' timeslot to talk which is 30 minutes' presentation and 10 minutes' discussion
- 3. Invited speaker(s) has in total 20 minutes' timeslot to talk which is 15 minutes' presentation and 5 minutes' discussion
- 4. General speaker(s) has in total 15 minutes' timeslot to talk which is 10 minutes' presentation and 5 minutes' discussion
- 5. When registering your attendance at ICDM 2019 front desk, all oral presenter(s) are required to submit their power point in PDF., PPT., or PPTX., only
- 6. The file name should indicate your schedule such as day (Day1), room (Room1), type of presenter (General), and abstract number, for example:

Keynote speaker	Day1_Room1_Keynote_ABS-1.pptx,		
Invited speaker	Day1_Room1_Invited_ABS-1.pptx,		
General speaker	Day1_Room1_General_ABS-1.pptx		













 Oral presenter(s) must submit their short paper for about 4-6 pages and follow the IOP template before 15 September 2019 (WILL NOT BE EXTENDED)

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- 1. Poster should be prepared on A0 size (841 x 1189 mm) in a portrait format.
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- Poster presenter(s) must submit their short paper for about 4-6 pages and follow the IOP template before 15 September 2019 (WILL NOT BE EXTENDED)















## **EXCURSION**

## CANDI BOROBUDUR TOUR 3 September 2019

## The 7<sup>th</sup> International Conference on DV-Xα Method (ICDM 2019) Grand Candi Hotel, Semarang, INDONESIA

- CANDI BOROBUDUR tour is a free tour sponsored by PT. UPGRI TOUR
- 2. All ICDM 2019 participants are recommended to join this activity to enjoy the wonderful Indonesia.
- In order to get the best services from PT. UPGRI TOUR, it is very important to make reservation through this link <a href="https://forms.gle/NhWZmoF2rmcGtD81A">https://forms.gle/NhWZmoF2rmcGtD81A</a> before 24 August 2019.
- 4. Since CANDI BOROBUDUR is a holly temple, visitor shall adhere to the dress code. Visitor may wear cool loose clothing that cover up your shoulders and knees. Wear pants as the steps leading to the top of the temple are high and not suited to skirts. Comfortable footwear is also a must.















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## **PAPER • OPEN ACCESS**

# Water Quality in the Maintenance of *Oreochromis niloticus* through Environmentally Friendly Biofloc Technology

To cite this article: Endah Rita Sulistya Dewi et al 2020 IOP Conf. Ser.: Mater. Sci. Eng. 835 012008

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# Water Quality in the Maintenance of *Oreochromis niloticus* through Environmentally Friendly Biofloc Technology

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Abstract. This Population growth that continues to increase demands continuous availability of food. Aquaculture is one of the sectors of food production which has the highest growth rate in the world. Facing this opportunity, aquaculture is faced with several challenges related to limited natural resources such as water and land, as well as waste water from aquaculture. Furthermore, the application of best aquaculture practices in aquaculture product certification requires environmentally friendly aquaculture practices. *Oreochromis niloticus tilapia* is a type of freshwater consumption fish and is now a popular pet fish in freshwater ponds in Indonesia. This study aims to analyze water quality in the maintenance of Tilapia through environmentally friendly Biofloc technology. This research method was designed in the form of Research and Development. The results showed that the water quality was proper for pond operation using minimal water exchange, the development of dense microbial populations through the management of microbial populations could control the concentration of ammonia in the water. Bacteria in ponds form biofloc, producing microbial proteins that make it possible to recycle unused feed protein, so as to minimize pollution.

Keywords: Biofloc, Oreochromis niloticus, Environment Friendly

## 1. Introduction

Aquaculture is a form of maintenance and breeding of various kinds of aquatic animals or plants that use water as its main component. Common activities include fish cultivation, shrimp cultivation, oyster cultivation, seaweed cultivation (algae).

Aquaculture is an activity to produce aquatic biota (organism) in a controlled environment in order to get profit. In the next two decades, it is estimated that the demand for fish or non-fish will double due to the increase in world population. No doubt, aquaculture is a very reliable industry. It is estimated that in 2020, aquaculture will produce more than 68 million tons, reaching 40% of global seafood production [1].

Tilapia (*Oreochromis niloticus*) is a cheap source of animal protein for human consumption. Fish farming can be done in ponds or rearing tanks. In the process of growth, protein metabolism by aquatic organisms generally produces ammonia as a result of excretion. At the same time, the protein in feces and inedible feed will be broken down by bacteria into the same product, thus the more intensive a cultivation activity will be followed by the higher concentration of nitrogen compounds especially ammonia in water [2-3].

The high organic waste from artificial feed (pellets) and feces resulting from intensive fish maintenance will cause buildup and sedimentation at the bottom of the maintenance water media, so a

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decomposition process is needed. If not decomposed the maintenance media will be decomposed anaerobically by anaerobic bacteria then form toxic gases such as sulfuric acid, nitrite, and ammonia and have a negative impact on the metabolism of aquatic organisms to death. To reduce organic waste and will be discharged into public waters, water quality management is needed so that the maintenance media remain in good condition. One of the efforts is a biological approach by utilizing bacterial activity to accelerate the process of decomposition of organic waste.

Along with the development of technology through a biological approach, biofloc technology has been applied to maintain the quality of aquaculture. Biofloc technology is a technology to use both heterotrophic and autotrophic bacteria that can convert organic waste intensively into flock-shaped microorganisms, which can then be utilized by fish as a food source [4-5]. Within the floc there are several forming organisms such as bacteria, plankton, fungi, algae, and suspended particles that affect the structure and nutrient content of biofloc, but the bacterial community is the most dominant microorganism in floc formation in biofloc [6].

Biofloc technology or active suspension technique, uses constant aeration to enable the process of aerobic decomposition and keep bacterial flocks in suspension [7]. In this system heterotrophic bacteria that grow with high density function as bioreactors that control water quality especially N concentrations as well as a source of protein for the organisms that are kept. Furthermore according to [6], states that the formation of biofloc by heterotrophic bacteria generally aims to increase nutrient utilization, avoid environmental stress and predation.

This research is important to assess the efficiency of water use, ammonia content in water, the use of nutrients as natural food and the reduction of waste pollution in tilapia fish farming. It is expected that perpetrators of aquaculture will continue to prioritize the use of science and technology in the management of sustainable aquaculture businesses.

## 2. Methods

This research is a research development (R & D) . The development procedure uses the Borg and Gall model. Biofloc technology application is also carried out in this activity, namely making biofloc pools, preparing water media, growing floc, feeding management and water quality management.



Figure 1. Biofloc Ponds

The application of biofloc technology is carried out in a round tarpaulin pond with a diameter of 150 cm, height, 100 cm. Maintenance water media is 1.5 m³ and fish density is 300 fish/m³. At the beginning before the fish were stocked, probiotics were given, namely EM4 floc forming at a dose of 5 cc/m³. The addition of probiotic bacteria was carried out along with the accumulation of feed given in the maintenance media for 42 maintenance days and the length of the fish was measured at the beginning and the end of maintenance. During maintenance measured water quality including ammonia, temperature, DO, and pH was carried out on days 0, 21 and 42.

## 3. Results and discussion

From the results of the study water quality data obtained in the measurement period are as follows: Table 1. Data on Biofloc Pond Water Quality in Tilapia Maintenance

Parameters	Day 0	Day 21	Day 42
Ammonia	0.015 mg / L	0.02 mg / L	0.013 mg / L
Temperature	26°C	28°C	28°C
DO	5.2 mg / L	8.4 mg / L	8.57 mg / L



Next, the ammonia content for 42 days, with sampling on day 0, day 21 and day 42, is presented in Figure 2.

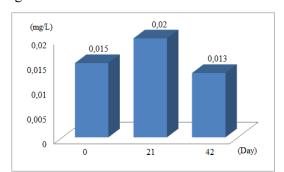


Figure 2. Ammonia Content in Biofloc Ponds

From this graph, it can be seen the average ammonia content of 0.016 mg / L, which means that the ammonia content in the pond is still below the quality standard. This condition can occur due to bacteria that can break down waste from fish, namely the Nitrosomonas bacteria, which convert Ammonia into Nitrites, Nitrites are then converted into Nitrates by Nitrobacter bacteria. According to [8] requirements, the maximum limit of ammonia levels for fish farming activities is <0.02 mg / L.

By [9] asserted that decomposition of ammonia by microbes can be done by deamination process. Deamination is the process of dismantling proteins into amino acids, then amino acids are broken down into ammonia and some other substances by the bacteria producing urease enzymes, with this enzyme urea can be broken down into ammonium carbonate, while ammonium carbonate is easily broken down into ammonia, carbon dioxide and water, also confirmed by [10] that the urease enzyme is the only catalyst enzyme in hydrolyzing urea. [11] added that the genus Bacillus is a microbe from a class of bacteria that is able to synthesize urease well in waters.

The need for good water quality in intensive fish maintenance requires an environmentally friendly technology so that the low organic matter in the maintenance media and the low waste that is discharged into public waters, in this case biofloc technology can provide a solution.

Broadly speaking, intensive maintenance of Tilapia with biofloc technology is more effective than without biofloc technology. And some supporting parameters such as temperature, DO, and pH are still within the maintenance threshold of tilapia. Provision of probiotics such as EM4 (Effective Microorganisms 4) has an important meaning in maintaining water quality by the process of breaking down waste materials into more useful organic matter. According to the opinion of [12] which states EM4 contains fermented and synthetic microorganisms consisting of Lactic Acid bacteria (*Lactobacillus sp*), Photosentetic Bacteria (*Rhodopseudomonas sp*), *Actinomycetes sp*, *Streptomyces sp* and Yeast (yeast) ) and cellulose decomposers.

[13] said that EM (Effective Microorganisms) consists of photosynthetic bacteria, lactic acid bacteria, actinomicetes, yeast and fermented fungi. Photosynthetic bacteria form beneficial substances that produce amino acids, nucleic acids and bioactive substances derived from harmful gases and function to bind nitrogen from the air. Lactic acid bacteria function to ferment organic material into lactic acid, accelerate the overhaul of organic matter, lignin and cellulose, and suppress pathogens with lactic acid produced. Actinomicetes produce anti-microbial substances from amino acids produced by photosynthetic bacteria. Yeast produces antibiotic substances, produces enzymes and hormones, yeast secretion becomes a substrate for effective microorganisms of lactic acid bacteria actinomycetes. Fermentation fungi are also able to break down organic matter quickly which produce anti-microbial ester alcohol, and eliminate the foul odor.

These microbes also play a role in floc formation. The formation of flocks in the pool can be seen with the characteristics of the pool does not smell, the color of the flocks in the pool is green which indicates in the pool more phytoplankton is formed.

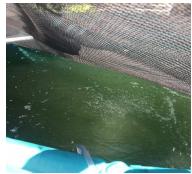


Figure 3. Floc formation

Concentrations of temperature, DO, and pH in each treatment ranged from 26-28°C; 5.2-8.57 mg / L; and 6-7. The three parameters show the results in the maintenance media are within reasonable limits for the growth of tilapia. Temperature requirements according to [8] 25-32°C as well as (DO) dissolved oxygen is within the proper limits for the growth of tilapia, according to the requirements of [8] SNI, DO is a minimum of 3 mg / L tilapia can still grow well at dissolved oxygen 5.2-8.57 mg / L. The pH concentration of water in the pond is within a reasonable limit for the growth of tilapia, ranging from 6-7 while [8] requirements are 6.5-8.5.

Ammonia's toxicity to aquatic animals is very dependent on pH, temperature and salinity. At high pH the NH3 levels will rise, and vice versa. When ammonia levels are high, the ability of fish to excrete ammonia is reduced. This causes an increase in ammonia levels in the blood and body tissues. This will increase blood pH levels and have a detrimental effect on enzyme sharing reactions and membrane stability. Negative effects include damage to the gills, reducing the capacity of blood to carry oxygen and histological damage to red blood cells [14]. From the results of observations of Ammonia (NH3) in ponds during the study containing ammonia with an average concentration of 0.016 mg / L. This proves that the role of flocks in ponds is able to maintain ammonia concentration during the tilapia aquaculture process. This condition is in accordance with the statement of [15] if the level of ammonia in the waters contained in an amount that is too high is greater than 1 mg / L can not be suspected of pollution.

## 4. Conclusion

- 1. Ammonia levels in biofloc ponds contain ammonia with an average concentration of 0.016 mg/L, still below the quality standard.
- 2. Water quality in biofloc ponds is declared feasible during maintenance of Tilapia.
- 3. Provision of EM4 forms biofloc and produces microbial proteins that play a role in recycling unused feed proteins, so as to minimize pollution.

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