

マッチングワークショップ2022

Matching Workshop 2022

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Current Research Theme

Laboratory general theme:

- First-principles approach to structure and dynamics at surface/interface
- Physics and Chemistry

Current Research theme:

Computational modelling fuel cell catalyst based on metal-oxides: **Zirconia (ZrO_2) surface** (currently)

Background

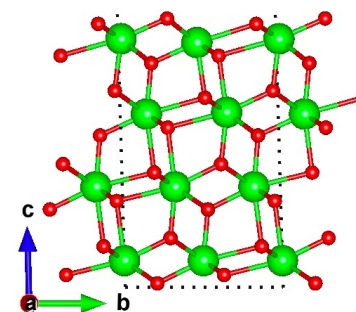
Platinum (Pt)-based fuel cell catalyst is promising but Pt has issues: **high cost, limited availability, and low chemical stability.**

Oxide catalyst is used as the alternative: **lower cost, high chemical stability, and higher oxygen reduction reaction (ORR) catalyst activity** than that of Pt.

What are we doing?

Performing a computational study using density-functional theory (DFT) and the computational hydrogen electrode model to investigate the ORR

Tools: **Quantum Espresso** (www.quantum-espresso.org/)



Green: Zr
Red: O

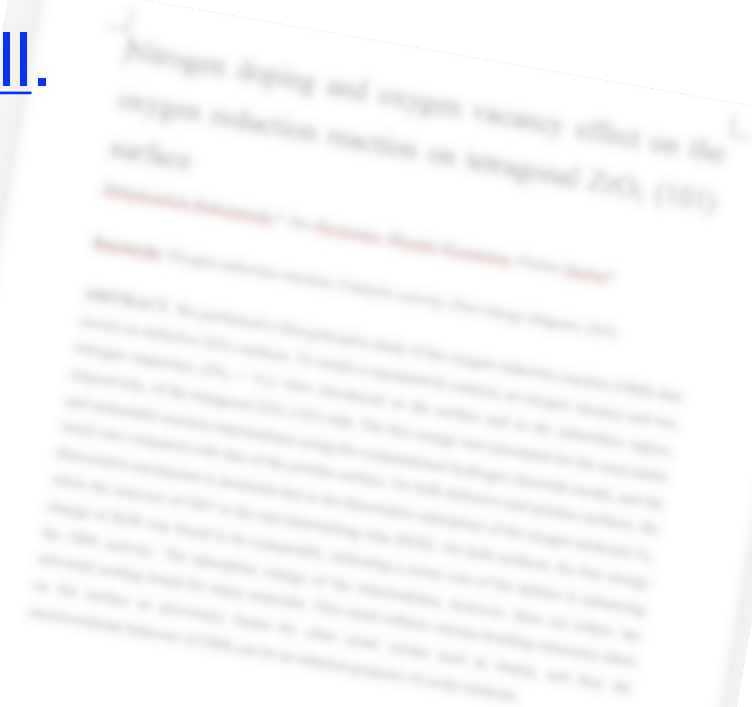
Current Research Theme

Expected results

- Effect of structural modification of the oxide surface (by modelling) on the catalyst activity.
- Physical properties of intermediates in elementary step of ORR, such as energy and structural configurations.
- New insight of oxide catalyst for fuel cell.

Outputs:

- Peer-reviewed publications
- Conferences/meetings



Higher educations and experiences

Higher Educations

- **Bachelor Degree (B.Sc/S.Si):** Sebelas Maret University, Indonesia (Major: Physics)
- **Master Degree (M.Sc/M.Si):** Bandung Institute of Technology, Indonesia
- **Doctoral Degree (Dr):** Bandung Institute of Technology, Indonesia

Research Experiences

- **Short-Term Visiting Trainee:** Solid-State Quantum Transport Group, Department of Physics, Graduate School of Science, Tohoku University (2015). Host: Prof. Yoshiro Hirayama (平山 祥郎)
- **Visiting Researcher:** College of Science and Technology, Nihon University (2016). Host: Prof. Kouichi Takase (高瀬 浩一)
- **Postdoctoral Researcher:** Department of Physics, Bandung Institute of Technology (2018-2020). Host: Prof. Yudi Darma

Scientific Journal Referee Experiences

Journal of Materials Science (Springer Nature): 09/2020, 12/2021, 05/2022 (3 times)

<https://www.springer.com/journal/10853>

Journal of Multidisciplinary Applied Natural Science: 11/2021 (1 time)

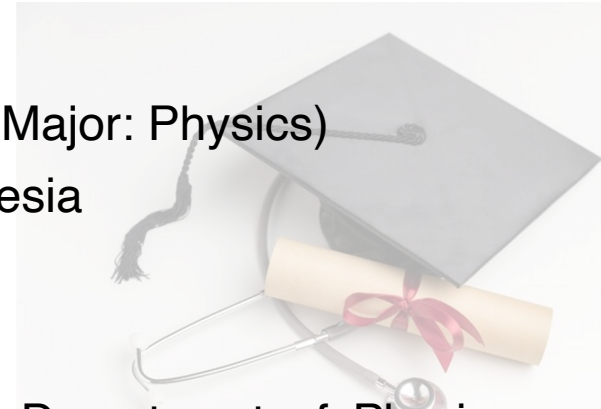
<https://journal.pandawainstitute.com/index.php/jmans/index>

Journal of Science and Applicative Technology: 10/2019, 04/2020 (2 times)

<https://journal.itera.ac.id/index.php/jsat>

ALCHEMY Jurnal Penelitian Kimia (Chemistry Research Journal): 08/2021 (1 time)

<https://jurnal.uns.ac.id/alchemy>



Publications

International publications: 31

Most important publications:

Shibghatullah Muhammady, Inge Magdalena Sutjahja, Andriwo Rusydi, Toto Winata, Kouichi Takase, Yudi Darma, “Unrevealed electronic and optical properties of the layered oxychalcogenides (LaO)CuCh (Ch = S, Se, Te): A density-functional study”, *Japanese Journal of Applied Physics*, **56**(12), 121201 (2017) DOI: [10.7567/JJAP.56.121201](https://doi.org/10.7567/JJAP.56.121201)

Shibghatullah Muhammady, Yudhi Kurniawan, Seiya Ishiwata, Awabaikeli Rousuli, Toshiki Nagasaki, Shogo Nakamura, Hitoshi Sato, Atsushi Higashiya, Atsushi Yamasaki, Yoshiaki Hara, Andriwo Rusydi, Kouichi Takase, Yudi Darma, “Electronic and thermoelectric properties of layered oxychalcogenides (BiO)CuCh (Ch = S, Se, Te)”, *Inorganic Chemistry*, **57**(16), 10214-10223 (2018) DOI: [10.1021/acs.inorgchem.8b01396](https://doi.org/10.1021/acs.inorgchem.8b01396)

Shibghatullah Muhammady, Adelya S. Erlyanti, Rena Widita, Yudi Darma, “Investigation of structural and electronic properties by pnictogen substitution in the layered oxypnictides (LaO)ZnPn (Pn = P, As, Sb)”, *International Journal of Quantum Chemistry*, **120**(3), e26090 (2020) DOI: [10.1002/qua.26090](https://doi.org/10.1002/qua.26090)

Shibghatullah Muhammady, Rena Widita, Yudi Darma, “Influence of Ch substitution on structural, electronic, and thermoelectric properties of layered oxychalcogenides (La_{0.5}Bi_{0.5}O)CuCh (Ch = S, Se, Te): a new insight from first principles”, *RSC Advances*, **10**(46), 27481-27491 (2020) DOI: [10.1039/D0RA05187J](https://doi.org/10.1039/D0RA05187J)

RSC Advances

PAPER

Check for updates

Cite this RSC Adv., 2020, 10, 27481

Influence of Ch substitution on structural, electronic, and thermoelectric properties of layered oxychalcogenides (La_{0.5}Bi_{0.5}O)CuCh (Ch = S, Se, Te): a new insight from first principles

Shibghatullah Muhammady, Rena Widita and Yudi Darma

We study the structural, electronic, and thermoelectric properties of p-type layered oxychalcogenides (La_{0.5}Bi_{0.5}O)CuCh (Ch = S, Se, Te) from first principles. Ch substitution from S to Te enhances the local-symmetry distortions (LSD) in CuCh, and (La_{0.5}Bi_{0.5}O)CuCh, where the LSD in (La_{0.5}Bi_{0.5}O)CuCh is more pronounced. The LSD in CuCh, tetrahedra comes from the possible pseudo-Jahn-Teller effect, indicated by the degeneracy-split t_{2g} and e_g states of Cu 3d⁹ orbitals. The Ch substitution decreases bandgap from 0.520 eV (S) to 0.443 eV (Se) to 0.394 eV (Te) for Ch = S, Se, Te, respectively, implying the increasing carrier concentration and electrical conductivity. The split-off energy at Z and Γ points are also increased by the substitution. The valence band shows deep O 2p states in the electron-confined (LaO)Cu²⁺ layers, which is essential for thermoelectricity. (La_{0.5}Bi_{0.5}O)CuCh provides the largest thermoelectric power from the Seebeck coefficient and the carrier concentration, which mainly come from Te 5p, Bi 6p, Cu 3d_{xy}, and Cu 3d_{yz} states. The valence band shows the partial hybridization of t_{2g} and Ch p states, implied by the presence of nonbonding valence t_{2g} states. This study provides new insights, which predict experimental results and are essential for novel functional device applications.

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rsc/advances

Recent/planned conferences/meetings/symposium: As a presenter

JPS Autumn Meeting 2022 (日本物理学会2022秋季大会) on 12-15 September 2022 at Tokyo Institute of Technology (東京工業大学). Organizer: The Physical Society of Japan (日本物理学会). <https://www.jps.or.jp/english/meetings-and-awards/autumn/autumn-meeting-index.html>.

The 241st ECS Meeting on 29 May – 2 June 2022 in Vancouver in British Columbia, Canada (Hybrid) (Symposium code: I03-1517, Abstract no.: 157379, *Digital Poster*). ecs.confex.com/ecs/241/meetingapp.cgi

The 19th International Union of Materials Research Society – International Conference in Asia (IUMRS – ICA) on 31 October – 2 November 2018 in Bali, Indonesia. (Symposium code: CMMS-O2, EasyChair ID: 60). <http://mrs-ina.org/iumrs-ica2018/>

The 9th International Conference on Physics and Its Applications (ICOPIA) on 14 August 2018 in Solo, Indonesia (Presentation code: M25, EasyChair ID: 109). <https://icopia2018.mipa.uns.ac.id/>.

The 7th Nanoscience and Nanotechnology Symposium (NNS) on 22-24 October 2017 in Bandung, Indonesia. (Presentation code: G1.4). <https://fmipa.itb.ac.id/id/event/7th-nanoscience-and-nanotechnology-symposium-nns-2017/>.