

# Ryan Lacdao Arevalo

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<b>Education</b>	<b>Ph.D. Quantum Engineering Design</b> , Osaka University, Japan, 2015 <ul style="list-style-type: none"><li>• Nanotechnology Summer School, Karlsruhe Institute of Tech., Germany, 2014</li><li>• Junior Research Fellowship, University College London, U.K., 2013</li></ul> <b>Master of Engineering</b> , Osaka University, Japan, 2012 <b>Master of Science in Physics</b> , De La Salle University, 2010 <b>BSE Physics &amp; Technology</b> (Magna Cum Laude), Philippine Normal University, 2006
<b>Research Interests</b>	<b>Computational Catalysis / Materials Modelling and Simulation</b> Methane Activation, Carbon Dioxide Conversion, Water Splitting, Electrochemical Reactions for Energy Conversion
<b>Work Experience</b>	<b>University of Limerick, Ireland</b> <ul style="list-style-type: none"><li>• Marie Skłodowska-Curie Fellow (2021-present)</li><li>• Postdoctoral Researcher (Mar. 2021–Sep. 2021)</li></ul> <b>De La Salle University, Manila, Philippines</b> <ul style="list-style-type: none"><li>• Associate Professorial Lecturer (2015–2016, 2020–2021)</li></ul> <b>National Institute of Technology, Akashi College, Japan</b> <ul style="list-style-type: none"><li>• Specially-Appointed Assistant Professor (2016–2019)</li></ul> <b>Philippine Normal University, Manila, Philippines</b> <ul style="list-style-type: none"><li>• Deputy Dean, College of Flexible Learning and e-PNU (Jan.–Jul. 2016)</li><li>• Physics Faculty (2006–2010; on non-binding study leave: 2011–2015)</li></ul>
<b>Scholarships / Grants / Awards (Selected)</b>	<b>Marie Skłodowska-Curie COFUND Fellowship</b> , University of Limerick, 2021 <b>Balik Scientist Program</b> , Host: University of San Carlos, Cebu, 2020-2021 <b>Murata Science Foundation</b> , Travel Grant to Washington D.C., U.S.A., 2017 <b>Research Citations Award</b> , Philippine Normal University, 2016 <b>Outstanding Faculty Award</b> , Faculty of Sci. Tech. Math., Phil. Normal Univ., 2016 <b>Robert Bosch Stiftung</b> , Summer School in Germany, 2014 <b>Thomas Young Centre Junior Research Fellowship</b> , UCL, London, U.K., 2013 <b>Marubun Research Promotion Foundation</b> , Travel Grant to Cambridge, U.K., 2013 <b>Monbukagakusho Scholarships</b> , 2010–2012 (Master's Degree), 2012–2015 (Doctorate)
<b>Professional Organizations</b>	<b>National Research Council of the Philippines</b> , Member (2020-present) <b>Royal Society of Chemistry</b> , Associate Member (2013-2019), Member (2019-present) <b>The Physical Society of Japan</b> , Member (2016-2018) <b>American Physical Society</b> , Member (2011-2017)
<b>License</b>	<b>Professional Teacher</b> , Licensure Examination for Teachers, 2006, Rating: 88.20%

## **PUBLICATIONS**

### **Refereed ISI-Indexed Journals**

1. R.L. Arevalo, S.M. Aspera, R.E.S. Otadoy, H. Nakanishi, H. Kasai, *Adsorption of CH<sub>4</sub> and SO<sub>2</sub> on unsupported Pd<sub>1-x</sub>M<sub>x</sub>O(101)*, *Catalysis Letters* 150 (2020) 1870.
2. R.L. Arevalo, S.M. Aspera, H. Nakanishi, *Sulfation of a PdO(101) methane oxidation catalyst: Mechanism revealed by first principles calculations*, *Catalysis Science & Technology* 9 (2019) 232.
3. R.L. Arevalo, S.M. Aspera, H. Nakanishi, H. Kasai, S. Yamaguchi, K. Asazawa, *Adsorption of carbonylhydrazide on Au(111) and Au<sub>3</sub>Ni(111) surfaces*, *Catalysis Letters* 148 (2018) 1073.
4. R.L. Arevalo, S.M. Aspera, M.C.S. Escaño, H. Nakanishi, H. Kasai, *Tuning methane decomposition on stepped Ni surface: Role of subsurface atoms in catalyst design*, *Scientific Reports* 7 (2017) 13963.
5. R.L. Arevalo, S.M. Aspera, M.C.S. Escaño, H. Nakanishi, H. Kasai, *First principles study of methane decomposition on B5 step-edge type site of Ru surface*, *Journal of Physics: Condensed Matter* 29 (2017) 18400.
6. R.L. Arevalo, S.M. Aspera, M.C.S. Escaño, H. Nakanishi, H. Kasai, *Ru-catalyzed steam methane reforming: Mechanistic study from first principles calculations*, *ACS Omega* 2 (2017) 1295.
7. R.L. Arevalo, M.C.S. Escaño, H. Kasai, *First-principles study of nitric oxide oxidation on Pt(111) versus Pt overlayer on 3d transition metals*, *Journal of Vacuum Science and Technology A* 33 (2015) 021402.
8. R.L. Arevalo, K. Oka, H. Nakanishi, H. Kasai, H. Maekawa, K. Osumi, N. Shimazaki, *Oxidation of NO on Pt/M (M = Pt, Co, Fe, Mn): A first-principles density functional theory*, *Catalysis Science and Technology* 5 (2015) 882.
9. R.L. Arevalo, M.C.S. Escaño, H. Kasai, *Mechanistic insight into the Au-3d metal alloy-catalyzed borohydride electro-oxidation: From electronic properties to thermodynamics*, *ACS Catalysis* 3 (2013) 3031.
10. R.L. Arevalo, M.C.S. Escaño, H. Kasai, *Computational mechanistic study of borohydride electrochemical oxidation on Au<sub>3</sub>Ni(111)*, *The Journal of Physical Chemistry C* 117 (2013) 3818.
11. R.L. Arevalo, M.C.S. Escaño, A.Y.-S. Wang, H. Kasai, *Structure and stability of borohydride on Au(111) and Au<sub>3</sub>M (M = Cr, Mn, Fe, Co, Ni)*, *Dalton Transactions* 42 (2013) 770.
12. R.L. Arevalo, H. Kishi, A.A.B. Padama, J.L.V. Moreno, H. Kasai, *Substrate dependence of Pt<sub>4</sub> electronic properties*, *Journal of Physics: Condensed Matter* 25 (2013) 222001. (*IOP Select Article*)
13. R.L. Arevalo, M.C.S. Escaño, E. Gyenge, H. Kasai, *A theoretical study of the structure and stability of borohydride on 3d transition metals*, *Surface Science* 606 (2012) 1954.
14. R.L. Arevalo, M.C.S. Escaño, H. Kasai, *First principles study on the adsorption and dehydrogenation of borohydride on Mn(111)*, *e-Journal of Surface Science and Nanotechnology* 9 (2011) 257.
15. R.L. Arevalo, R.F. Pobre, *DFT and cluster model investigation on the adhesion of polyethylene terephthalate on metals*, *e-Journal of Surface Science and Nanotechnology* 9 (2011) 251.
16. S.M. Aspera, R.L. Arevalo, B. Chantaramolee, H. Nakanishi, H. Kasai, *PdRuIr ternary alloy as an effective NO reduction catalyst: insights from first-principles calculation*, *Physical Chemistry Chemical Physics* 23 (2021) 7153.
17. S.M. Aspera, R.L. Arevalo, H. Nakanishi, H. Kasai, S. Sekine, H. Kawai, *Vanadium doped Polyoxometalate: Induced active sites and increased hydrogen adsorption*, *Journal of Physics: Condensed Matter* 32 (2020) 195001.
18. S.M. Aspera, R.L. Arevalo, H. Nakanishi, H. Kasai, *First principles study of surface stability and segregation of PdRuRh ternary metal alloy system*, *Surface Science* 671 (2018) 51.
19. S.M. Aspera, R.L. Arevalo, K. Shimizu, R. Kishida, K. Kojima, N.H. Linh, H. Nakanishi, H. Kasai, *First principles calculation of transition metal binary alloys: Phase stability and surface effect*, *Journal of Electronic Materials* 46 (2017) 3776.
20. J.L.V. Moreno, R.L. Arevalo, M.C.S. Escaño, A.A.B. Padama, H. Kasai, *A theoretical study on the adsorption of CO<sub>2</sub> on*

- CuO(110) surface*, Journal of Physical Society of Japan 84 (2015) 015003.
21. M.C.S. Escano, R.L. Arevalo, E. Gyenge, H. Kasai, *Electrocatalysis of borohydride: a review of density functional theory approach combined with experimental verification*, Journal of Physics: Condensed Matter 26 (2014) 353001.
  22. M.C.S. Escaño, R.L. Arevalo, E. Gyenge, H. Kasai, *First-principles study of borohydride adsorption properties on osmium nanoparticles and surfaces: Understanding facet, size effects and local sites*, Catalysis Science & Technology 4 (2014) 1301.
  23. M.C.S. Escaño, R.L. Arevalo, E. Gyenge, H. Kasai, *Water co-adsorption and electric field effects on borohydride structures on Os(111) by first-principles calculations*, Journal of Alloys and Compounds 580 (2013) S6.
  24. B. Chantaramolee, S.M. Aspera, R.L. Arevalo, E.F. Arguelles, R. Kishida, A.A.B. Padama, H. Kasai, H. Nakanishi, *Surface compositions of Pt-Pd/Pd(111) alloys in the presence of O and OH during oxygen reduction reaction: A first principles study*, Journal of the Physical Society of Japan 88 (2019) 044820.
  25. R. Kishida, A.G. Saputro, R.L. Arevalo, H. Kasai, *Effects of introduction of  $\alpha$ -carboxylate, N-methyl, and N-formyl groups on intramolecular cyclization of o-quinone amines: Density functional theory-based study*, International Journal of Quantum Chemistry 7 (2017) 23.
  26. H. Kishi, A.A.B. Padama, R.L. Arevalo, J.L.V. Moreno, H. Kasai, M. Taniguchi, M. Uenishi, H. Tanaka, Y. Nishihata, *A theoretical study of the reactivity of Cu<sub>2</sub>O(111) surfaces: the case of NO dissociation*, Journal of Physics: Condensed Matter 24 (2012) 262001. (*IOP Select Article*)
  27. A.A.B. Padama, H. Kishi, R.L. Arevalo, J.L.V. Moreno, H. Kasai, M. Taniguchi, M. Uenishi, H. Tanaka, Y. Nishihata, *NO dissociation on Cu(111) and Cu<sub>2</sub>O(111) surfaces: a density functional theory based study*, Journal of Physics: Condensed Matter 24 (2012) 175005.
  28. M.C.S. Escaño, E. Gyenge, R.L. Arevalo, H. Kasai, *Reactivity descriptor for borohydride interaction with metal surfaces*, The Journal of Physical Chemistry C 115 (2011) 19883.
  29. R. Kishida, S. Ito, M. Sugumaran, R.L. Arevalo, H. Nakanishi, H. Kasai, *Density functional theory-based calculation shed new light on the bizarre addition of cysteine thiol to dopaquinone*, International Journal of Molecular Sciences 22 (2021) 1373.
  30. R. Kishida, H. Kasai, S.M. Aspera, R.L. Arevalo, H. Nakanishi, *Branching reaction in melanogenesis: The effect of intramolecular cyclization on thiol binding*, Journal of Electronic Materials 46 (2017) 3784.
  31. R. Kishida, H. Kasai, S.M. Aspera, R.L. Arevalo, H. Nakanishi, *Density functional theory-based first principles calculations of rhododendrol-quinone reactions: Preference to thiol binding over cyclization*, Journal of the Physical Society of Japan 86 (2017) 024804.
  32. W.T. Cahyanto, M.C. Escaño, H. Kasai, R.L. Arevalo, *Pt(111)-Alloy Surfaces for Non-Activated OOH Dissociation*, e-Journal of Surface Science and Nanotechnology 9 (2011) 352.
  33. T. Wakisaka, K. Kusada, D. Wu, T. Yamamoto, T. Toriyama, S. Matsumura, H. Akiba, O. Yamamuro, K. Ikeda, T. Otomo, N. Palina, Y. Chen, L.S.R. Kumara, C. Song, O. Sakata, W. Xie, M. Koyama, Y. Kubota, S. Kawaguchi, R.L. Arevalo, S.M. Aspera, E.F. Arguelles, H. Nakanishi, H. Kitagawa, *Rational Synthesis for a Noble Metal Carbide*, Journal of the American Chemical Society 142 (2020) 1247.

#### Refereed Non-ISI-Indexed Journals

1. R.L. Arevalo, *Quantum and atomic scale materials modeling in the Philippines: Status, challenges, and recommendations*, KIMIKA 31 (2020) 56.
2. R.L. Arevalo, M.C.S. Escaño, A.A.B. Padama, H. Kasai, *Adsorbate-induced demagnetization: Borohydride on magnetic substrates*, International Journal of Philippine Science and Technology 9 (2016) 10.
3. R.L. Arevalo, S.M. Aspera, R.E.S. Otadoy, H. Nakanishi, H. Kasai, *Role of water dissociation kinetics on Ni-catalyzed*

*atomic carbon conversion in a steam reforming environment: Which path to take?* Proceedings of the Samahang Pisikang Pilipinas, 2020.

4. R.L. Arevalo, S.M. Aspera, H. Nakanishi, H. Kasai, *DFT-guided design of catalysts for methane activation*, AIP Conference Proceedings 2040 (2018) 020004.
5. R.L. Arevalo, R.F. Pobre, *DFT calculation for the bandstructure of rutile SnO<sub>2</sub>*, Proceedings of 27<sup>th</sup> SPP National Physics Congress, 2009.
6. M.C.S. Escaño,\* R.L. Arevalo, H. Kasai, *Differentiating electro-catalytic reaction of hydride with respect to a non-Pt catalyst morphology based on first-principles: extended surfaces versus nanoparticles*, Technical Proceedings of the 2014 Clean Technology Conference and Trade Show, vol. 3, 2014, 380-383.
7. J.S. Gueriba,\* A.A.B. Padama, R.L. Arevalo, M. David, N. Arboleda, H. Kasai, *A first principles study of hydrogen interaction with Ca decorated SiCNT*, Proceedings of the DLSU Research Congress, vol. 3, 2015.

#### Patents

1. H. Nakanishi, H. Kasai, R.L. Arevalo, 耐硫黄被毒性を有するメタン浄化触媒 (Sulfur-poisoning resistant methane oxidation catalyst), Application No. 2019-173438, Publication No. 2021-049491 (Pending).
2. H. Nakanishi, H. Kasai, R.L. Arevalo, 耐コーキング作用を有するメタンの活性化触媒 (Methane activation catalyst with anti-coking property), Application No. 2017-129580, Publication No. 2019-010628, Patent Registration No. 特許第 6832010 号 (2021).

#### Book/Textbook

1. R.L. Arevalo, *General Physics 1*, Diwa Learning Systems Inc., 2016 (ISBN: 978-971-46-1069-9)
2. H. Kasai, A.A.B. Padama, B. Chantaramolee, R.L. Arevalo, *Hydrogen and Hydrogen-Containing Molecules on Metal Surfaces: Towards the Realization of Sustainable Hydrogen Economy*, Springer Nature Singapore Pte Ltd., 2020 (Hardcover ISBN:

978-981-15-6993-7; eBook ISBN: 978-981-15-6994-4)

#### Conference Abstracts (incomplete list)

\*Presenting Author

1. R.L. Arevalo,\* H. Nakanishi, S.M. Aspera, H. Kasai, *Sulfation of PdO(101) Methane Oxidation Catalyst: Mechanism Revealed by First Principles Calculations*, Abstracts of the Annual Meeting of the Physical Society of Japan, 2019.
2. R.L. Arevalo,\* H. Nakanishi, S.M. Aspera, E.F. Arguelles, V. Khoirunisa, H. Kasai, *Methane decomposition on Ni surface: Towards designing non-coking catalysts for hydrocarbon reforming*, Abstracts of the Autumn Meeting of the Physical Society of Japan, 2018.
3. R.L. Arevalo,\* S.M. Aspera, H. Kasai, H. Nakanishi, S. Matsumura, *Methane activation on Ni surface: DFT-based insights into catalyst design*, Abstracts of the 8th Tokyo Conference on Advanced Catalytic Science and Technology, Yokohama, 2018
4. R.L. Arevalo,\* S.M. Aspera, H. Nakanishi, H. Kasai, *DFT-guided design of non-coking Ni-based catalysts for methane reforming*, Proceedings of the Japan-Germany Joint Symposium on Advanced Catalytic Materials and Characterization, Munich, June 2018.
5. R.L. Arevalo,\* S.M. Aspera, M.C.S. Escaño, H. Nakanishi, H. Kasai, *Tuning methane decomposition on stepped Ni surface: Role of subsurface atoms in catalyst design*, Abstracts of the 73<sup>rd</sup> Annual Meeting of the Physical Society of Japan, 2018.
6. R.L. Arevalo,\* S.M. Aspera, H. Nakanishi, H. Kasai, *How do Ru and Ni surface catalyze the decomposition of methane? New insights for catalyst design*, Abstracts of the 254<sup>th</sup> American Chemical Society National Meeting and Exposition, Washington DC, Aug. 2017.
7. R.L. Arevalo,\* S.M. Aspera, H. Nakanishi, H. Kasai, *How do Ru and Ni surface catalyze the decomposition of methane? New insights for catalyst design*, Proceedings of the UK-Japan Joint Symposium on

- Nanomaterials, Catalysis, and Hydrogen Research, Canterbury, Jul. 2017.
8. R.L. Arevalo,\* S.M. Aspera, H. Nakanishi, H. Kasai, *Catalysis of steam methane reforming: From electronic properties to thermodynamics*, Proceedings of the EMN Croatia Conference, Croatia, May 2017.
  9. R.L. Arevalo,\* S.M. Aspera, M.C.S. Escano, H. Nakanishi, H. Kasai, *How do Ru and Ni surfaces catalyze the steam reforming of methane?*, Abstracts of the 72<sup>nd</sup> Annual Meeting of the Physical Society of Japan, 2017.
  10. R.L. Arevalo,\* H. Kasai, *Rational Catalyst Design Approach to heterogeneous Catalysis: Oxidation of borohydride and nitric oxide*, Abstracts of the Kansai Thin Films and Surface Physics Seminar, 2014
  11. R.L. Arevalo, K. Oka, H. Nakanishi, H. Kasai, H. Maekawa, K. Osumi, N. Shimazaki, *NO oxidation on Pt/M (M = Pt, Co, Fe, Mn)*, Abstracts of the 55<sup>th</sup> Annual Symposium of the Vacuum Society of Japan, 2014.
  12. R.L. Arevalo,\* M.C.S. Escaño, H. Kasai, *Adsorbate-Induced Demagnetization: Borohydride on Magnetic Substrates*, Proceedings of the 19<sup>th</sup> Osaka University – De La Salle University Workshop, 2014
  13. R.L. Arevalo,\* M.C.S. Escaño, H. Kasai, *First-Principles Mechanistic Insights into the Au-3d Metal Alloy – Catalyzed Borohydride Electro-oxidation*, Proceedings of the International Symposium on Atomically Controlled Fabrication Technology, 2014.
  14. R.L. Arevalo,\* H. Kasai, *Borohydride oxidation on Au-3d metal alloys: Mechanistic study from first-principles calculations*, Proceedings of the Joint Annual Symposium of the Vacuum Society of Japan and the Surface Science Society of Japan, 2013.
  15. R.L. Arevalo,\* H. Kasai, *Borohydride oxidation on Au-3d metal alloys: Mechanistic study from first-principles calculations*, Proceedings of the International Symposia on Advancing the Chemical Sciences: Challenges in Chemical Renewable Energy (ISACS12), Cambridge, United Kingdom, 2013.
  16. R.L. Arevalo,\* M.C.S. Escaño, H. Kasai, *Structure and stability of borohydride on Au(111) and Au<sub>3</sub>M(111) (M = Cr, Mn, Fe, Co, Ni) surfaces*, Proceedings of the 53<sup>rd</sup> Annual Symposium of the Vacuum Society of Japan, Kobe, Japan, 2012.
  17. R.L. Arevalo,\* M.C.S. Escaño, H. Kasai, *Structure and stability of borohydride on Au(111) and Au<sub>3</sub>M(111) (M = Cr, Mn, Fe, Co, Ni) surfaces*, Proceedings of the Fifth International Symposium on Atomically Controlled Fabrication Technology, 2012.
  18. R.L. Arevalo,\* M.C.S. Escaño, H. Kasai, *Structure and stability of borohydride on Au(111) and Au<sub>3</sub>M(111) (M = Cr, Mn, Fe, Co, Ni) surfaces*, Proceedings of the International Symposium on Computics: Quantum Simulation and Design (ISC QSD), 2012.
  19. R.L. Arevalo,\* M.C.S. Escaño, H. Kasai, *Borohydride adsorption and interaction with OH on Mn(111)*, Proceedings of the International Symposium on Materials Science and Innovation for Sustainable Society (Eco-mates 2011).
  20. R.L. Arevalo,\* M.C.S. Escaño, H. Kasai, *Interaction of borohydride with 3d transition metals: a DFT study*, Proceedings of the Fourth International Symposium on Atomically Controlled Fabrication Technology, 2011.
  21. R.L. Arevalo,\* M.C.S. Escaño, H. Kasai, *Borohydride dehydrogenation and interaction with OH on Mn(111)*, Proceedings of the JSMS Symposium on Multiscale Materials Modeling, 2011.
  22. S.M. Aspera\*, R.L. Arevalo, B. Chantaramolee, H. Nakanishi, H. Kasai, *Computational Materials Design: Insights on catalyst design for methane dry reforming on Ni-based stepped surfaces*, Abstracts of the 2nd PAPS International 3-Day Research Conference, 2021.
  23. S.M. Aspera\*, R.L. Arevalo, B. Chantaramolee, H. Nakanishi, H. Kasai, *First principles analysis of NO dissociation on the quaternary alloy PdRuIrM (M = Ni, Co, Fe): Effect of the fourth metal alloy on surface reactivity*, Abstracts of the Autumn Meeting of the Physical Society of Japan, 2021.
  24. S.M. Aspera\*, R.L. Arevalo, B. Chantaramolee, H. Nakanishi, H. Kasai, *Ab initio analysis on the capability of PdRuIr ternary alloy as an NO reduction catalyst*, Abstracts of the 76<sup>th</sup> Annual Meeting of the Physical Society of Japan, 2021.

25. S.M. Aspera\*, [R.L. Arevalo](#), H. Nakanishi, H. Kasai, *PdRuIr ternary alloy as an effective NO reduction catalyst: Insights from first principles calculation*, Bulletin of the American Physical Society, APS March Meeting, 2021.
26. B. Chantaramolee\*, [R.L. Arevalo](#), S.M. Aspera, H. Nakanishi, H. Kasai, *First principles study of oxygen reduction reaction on Pt*, Abstracts of the 75<sup>th</sup> Annual Meeting of the Physical Society of Japan, 2020.
27. S.M. Aspera\*, [R.L. Arevalo](#), H. Nakanishi, H. Kasai, *On understanding ternary alloys: Third-metal effect of PdRuM (M=Rh, Ir) on NO reduction*, Proceedings of the Japan-Germany Joint Symposium on Advanced Catalytic Materials and Characterization, Munich, June 2018.
28. S.M. Aspera\*, [R.L. Arevalo](#), B. Chantaramolee, H. Nakanishi, H. Kasai, *NO reduction on ternary alloy PdRuM (M = Rh, Ir) catalysts using first principles calculations*, Proceedings of the 73<sup>rd</sup> Annual Meeting of the Physical Society of Japan, 2018.
29. S.M. Aspera\*, [R.L. Arevalo](#), B. Chantaramolee, H. Nakanishi, H. Kasai, *PdRuRh Ternary Alloy as NO Reduction Catalyst: A DFT-based First Principles Analysis*, Proceedings of the Physical Society of Japan Autumn Meeting, Sept. 2017.
30. H. Nakanishi, [R.L. Arevalo](#)\*, S.M. Aspera, H. Kasai, *Computational materials design of virtual noble metals*, Proceedings of the UK-Japan Joint Symposium on Nanomaterials, Catalysis, and Hydrogen Research, Canterbury, Jul. 2017.
31. S.M. Aspera\*, [R.L. Arevalo](#), H. Nakanishi, H. Kasai, *2D materials for fuel cell: Functionalization of graphitic carbon nitride for oxygen reduction reaction (ORR) application*, Proceedings of the UK-Japan Joint Symposium on Nanomaterials, Catalysis, and Hydrogen Research, Canterbury, Jul. 2017.
32. S.M. Aspera\*, [R.L. Arevalo](#), H. Nakanishi, H. Kasai, *Surface segregation and stability of PdRuM (M = Rh, Ir, Ni, Ag) ternary metal alloy surfaces through first principles-based studies*, Bulletin of the American Physical Society, APS March Meeting, 2017.
33. S.M. Aspera\*, [R.L. Arevalo](#), H. Nakanishi, H. Kasai, *First principles based studies of PdRuM (M=Rh, Ir, Ni, Ag) ternary metal alloy surfaces: Surface segregation and stability*, Proceedings of the 72<sup>nd</sup> Annual Meeting of the Physical Society of Japan, 2017.
34. H. Nakanishi\*, [R.L. Arevalo](#), S.M. Aspera, H. Kasai, *Quantum simulation for the motion of positive-muon in materials and its application for Mu-SR spin state analysis*, Proceedings of the International Workshop on Computational Science, Kanazawa University, 2017.
35. J.A.A. Abrea\*, J.J.Y. Lim, [R.L. Arevalo](#), R.E.S. Otadoy, A.C. Javier, *Dissociative H<sub>2</sub> adsorption on Pt/M (M = Mn, Fe, Co) bimetallic systems using density functional theory*, Abstracts of the 35<sup>th</sup> Philippine Chemistry Congress, 2021.
36. H. Nakanishi\*, S.M. Aspera, [R.L. Arevalo](#), 合金触媒表面における水素化反応の理論計算, Abstracts of the 第4回ハイドロジェノミクス研究会, 2021.
37. B. Chantaramolee, S.M. Aspera, [R.L. Arevalo](#), E.F. Arguelles, H. Kasai, H. Nakanishi, *Direct formaldehyde dissociation on (111) and (0001) surfaces*, Abstracts of the 76<sup>th</sup> Annual Meeting of the Physical Society of Japan, 2021.
38. H. Nakanishi, S.M. Aspera, [R.L. Arevalo](#), H. Kasai, *An international graduate school level collaborative program in NIT Akashi on cutting edge research and project developments*, Abstracts of the 14<sup>th</sup> International Symposium on Advances in Technology Education (ISATE2021), Finland, 2021.
39. H. Kasai, R. Kishida, [R.L. Arevalo](#), *Binding mechanism of L-cysteine to dopaquinone investigated by density functional theory-based calculation*, Abstracts of the Annual Meeting of the Japan Society of Vacuum and Surface Science, 2020.
40. R. Fajardo, J. Anthoniappen, [R.L. Arevalo](#), F.M. Ruiz, R.E. Otadoy, F. Buot, *Pyroelectric properties of Zirconium-doped BaTiO<sub>3</sub> solid solutions using X-ray diffraction and first principles calculations*, Proceedings of the Samahang Pisika ng Pilipinas, 2020.
41. B. Chantaramolee\*, S.M. Aspera, [R.L. Arevalo](#), H. Nakanishi, H. Kasai, *HCHO dissociation on Pt(111) and Rh(111)*,

- Proceedings of the Physical Society of Japan Autumn Meeting, Sept. 2017.
42. H. Kasai,\* R.L. Arevalo, M.C.S Escano, *Surface and interface as a foundation to realizing designer materials*, Proceedings of the Materials Research Society Fall Meeting 2015, Boston, 2015.
  43. H. Nakanishi,\* S.M. Aspera, R.L. Arevalo, H. Kasai, *An international graduate-school-level collaborative program in NIT Akashi on cutting edge research and project developments*, 14<sup>th</sup> International Symposium on Advances in Technology Education, Turku, Finland, Aug. 2020.
  44. H. Nakanishi,\* C.A. Pelotenia, R.L. Arevalo, S.M. Aspera, H. Kasai, *Sophisticated design of molecular bridge devices*, Proceedings of the Japan-Germany Joint Symposium on Advanced Catalytic Materials and Characterization, Munich, June 2018.
  45. H. Kasai, M.C.S. Escaño, R.L. Arevalo,\* *Platinum overlayer on 3d transition metals: Reactivity towards O<sub>2</sub> dissociation and NO oxidation*, Abstracts of the 14<sup>th</sup> International Conference on Atomic Layer Deposition, 2014
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