2025年度スーパーコンピューティングシステム

利用研究成果報告書

（2025年4月～2026年3月）

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Ⅲ．国際会議発表論文

＜ Proceeding　2025年＞

1. Exploration of stability, thermochemistry, and bonding of microhydrated N_2O clusters
   J. Phys. Conf. Ser.（International Conference on Innovative Materials 2024（ICIM-2024）21/11/2024 - 22/11/2024 Uzhavoor, India）, 2995（2025）Art.No.012012
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2. Atomistic insights into the role of solute interaction in phosphorus segregation at grain boundaries in α-Fe
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3. APLICAÇÃO DE TERMODINÂMICA COMPUTACIONAL PARA MAPEAMENTOS DE EQUILÍBRIO E ANÁLISE DE SÓLIDOS FORMADOS A PARTIR DE PROCESSOS CORROSIVOS EM ÁGUAS SALINAS
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4. MAPEAMENTO DA CURVA DE TRANSFORMAÇÃO DE FASE POR RESFRIAMENTO CONTÍNUO DE UM AÇO LAMINADO A FRIO NO SIMULADOR TERMOMECÂNICO GLEEBLE
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1. Atomistic study of grain boundary character influence on solute segregation in α-Fe: Symmetric tilt and twist grain boundaries
   CAMP-ISIJ, 39（2026）Art.No.198
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＜2025年＞

1. Machine Learning analysis of double perovskite B-site composition and band gap energy
   The Asia-Pacific International Conference on Perovskite, Organic Photovoltaics and Optoelectronics（IPEROP25）
   Kyoto University, Kyoto, Japan（2025.1.20-21）（Poster）
   Saho Kobayashi（Kajikawa）, Masanori Kaneko, Takahito Nakajima, Koichi Yamashita and Azusa Muraoka

2. Theoretical Study on Deep Levels Induced by Defect Structures in Sn/Ge Double Perovskite Solar Cell Materials Using First-Principles Calculations
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   Kyoto University, Kyoto, Japan（2025.1.20-21）（Poster）
   Mai Otake, Suzune Omori, Masanori Kaneko, Giacomo Giorgi, Koichi Yamashita and Azusa Muraoka

3. The Role and Impact of Vibronic Interactions on Charge Transfer Excitons in BTA-Based Nonfullerene Organic Solar Cells
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4. Implications of Fictive Temperature for MD-Simulated Silica Glass: with Respect to Experiments
   Symposium on Hyper-Ordered Structure Sciences in London
   Japan House London, London, UK（2025.1.29-31）No.P15s（Poster）
   Shunsuke Hiiro, Kazuro Kizaki, Liping Huang and Madoka Ono

5. Density Functional Theory Approaches for Modeling Heterogeneous Catalysis
   FHI-aims webinar Series: From Model to Mechanism in Heterogeneous Catalysis
   Online（2025.4.2-3）（Invited）
   Ray Miyazaki

6. Prediction of High-Frequency Dielectric Properties of Polymers Using Molecular Dynamics Simulations
   2025 MRS Spring Meeting & Exhibit
   Seattle, Washington, USA（2025.4.7-11）No.MT02.09.03（Oral）
   Masato Ohnishi, Koki Kitai, Yuta Yoshimoto, Yoshihiro Hayashi, Ryo Yoshida and Junichiro Shiomi

7. Modulating Charge Separation via Vibronic Coupling in Nonfullerene Organic Photovoltaics
   11th The Asia-Pacific Association of Theoretical and Computational Chemists（APATCC11）
   Kobe International Conference Center, Kobe, Hyogo, Japan（2025.4.21-25）
   No.1C2（Invited）
   Azusa Muraoka

8. Molecular Insight into the Adsorption and Conversion at the Liquid/Solid-Oxide Interface
   11th The Asia-Pacific Association of Theoretical and Computational Chemists（APATCC11）
   Kobe International Conference Center, Kobe, Hyogo, Japan（2025.4.21-25）
   No.2D5（Invited）
   Akira Nakayama

9. Materials Genes of CO2 Hydrogenation on Supported Cobalt Catalysts: an AI Approach Integrating Theoretical and Experimental Data
   11th The Asia-Pacific Association of Theoretical and Computational Chemists（APATCC11）
   Kobe International Conference Center, Kobe, Hyogo, Japan（2025.4.21-25）
   No.4B3（Invited）
   Ray Miyazaki, Kendra Belthle, Harun Tüysüz, Lucas Foppa and Matthias Scheffler

10. Turing Scheme for Catalysis and DigCat 3.0 – An Intelligent Digital Platform Powered by Ultra-Large-Scale Exp + Comput Data
    Seminar of the Chinese Academy of Sciences（CAS）
    China（2025.4.25）（Invited）
    Hao Li

11. Turing Scheme for Catalysis and DigCat 3.0 – An Intelligent Digital Platform Powered by Ultra-Large-Scale Exp + Comput Data
    The 2nd International Forum on AI 4 Materials
    Taiyuan, China（2025.4.26）（Plenary）
    Hao Li

12. Turing Scheme for Materials – An Intelligent Digital Platform Powered by Ultra-Large-Scale Exp + Comput Data
    The First National Conference on Surface and Interface Science of the Chinese Chemical Society
    Chengdu, China（2025.5.9-12）（Keynote）
    Hao Li

13. Shear-induced Surface Aromatization as a Super-lubricity Mechanism of Amorphous Carbon
    79th STLE Annual Meeting & Exhibition
    Atlanta, GA, USA（2025.5.18-22）（Oral）
    T. Kuwahara

14. Electronic structure in light-element-doped TiO_2 by all-electron GW calculation using TOMBO code
    AAPALI PSI-K 2025, International Conference on Density Functional Theory and Applications
    IISER Pune, India（2025.5.19-21）（Invited）
    Ryoji Sahara, Takashi Ishikawa, Kaoru Ohno, Kyosuke Ueda and Takayuki Narushima

15. Large Scale Reactive Molecular Dynamics Simulation of Catalyst Layer Structure with High Electrode Reaction Activity in Polymer Electrolyte Fuel Cell Cathode
    The 20th Japan-Korea Symposium on Catalysis（20JKSC）
    Yonago, Japan（2025.5.19-22）No.GO D16（Oral）
    Nobuki Ozawa, Kaito Mori, Tetsuya Nakamura and Momoji Kubo

16. Develop a Closed-Loop Framework for AI Materials Lab
    Seminar of Shenzhen Institute of Advanced Technology
    Shenzhen, China（2025.5.21）（Invited）
    Hao Li

17. Electronic structure calculation and machine learning prediction: extension from cantor-derived high entropy alloys
    Material Science: Modeling & Design in Action
    NIMS, Japan（2025.5.21-22）（Invited）
    Ying Chen, Tran Nguyen-Dung, Yibo Sun and Jun Ni

18. Theoretical study on the four-electron oxidation mechanism of cobalt oxide catalysts
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    Kyoto Terrsa（2025.5.23-28）No.PI-34（Poster）
    Azusa Muraoka, Narumi Fujiwara and Koichi Yamashita

19. Molecular insight into C-C bond cleavage of alkanes on Ru surfaces based on free energy landscape
    MQM2025
    Kyoto Terrsa（2025.5.23-28）No.PI-35（Poster）
    Kenshin Takei, Tatsushi Ikeda, Koki Muraoka and Akira Nakayama

20. Microscopic Structure and Proton Hopping Mechanisms at the Water/ZrO_2 Interface
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    Kyoto Terrsa（2025.5.23-28）No.PI-36（Poster）
    Tori Oishi, Tatsushi Ikeda and Akira Nakayama

21. Pt-Rh Thermodynamic Database using Neural Network Potential
    CALPHAD LII
    Paradise Hotel Busan, Busan, Korea（2025.5.25-30）No.TueOR1-3（Oral）
    A. Saengdeejing, R. Sahara, H. Kino and Toyohiro Chikyow

22. Empowering Future Women Researchers through Theoretical and Computational Chemistry in Solar Cell Research
    10th Japan-Taiwan-Thai workshop on Theoretical and Computational Chemistry 2025
    Kanazawa-Hakkei Campus of Yokohama City University, Yokohama, Japan（2025.5.31）（keynote）
    Azusa Muraoka

23. Non-adiabatic excited-state time-dependent *GW*（TDGW）molecular dynamics satisfying extended Koopmans' theorem
    TOMBO Workshop
    Yokohama, Japan（2025.5.31）（Invited）
    Aaditya Manjanath

24. Development of mechanoluminescence and multipiezo materials
    The 11th General Conference of the Asian Consortium on Computational Materials Science（ACCMS-11）
    Yokohama, Japan（2025.6.1-3）No.I-15（Invited）
    Chao-nan Xu

25. Time-dependent *GW* molecular dynamics – a new possible paradigm for an accurate description of dynamics of photochemical reactions
    The 11th General Conference of the Asian Consortium on Computational Materials Science（ACCMS-11）
    Yokohama, Japan（2025.6.1-3）No.I-22（Invited）
    Aaditya Manjanath, Muhammad Zakaria, Vannajan Lee, Ryoji Sahara, Kaoru Ohno and Yoshiyuki Kawazoe

26. Stability and novel ordered phases prediction in unclear fuel materials
    The 11th General Conference of the Asian Consortium on Computational Materials Science（ACCMS-11）
    Yokohama, Japan（2025.6.1-3）No.I-28（Invited）
    Ying Chen and Hua Yun Geng

27. Bayesian optimization with Gaussian process assisted by deep learning for material designs
    The 11th General Conference of the Asian Consortium on Computational Materials Science（ACCMS-11）
    Yokohama, Japan（2025.6.1-3）No.I-51（Invited）
    Shin Kiyohara

28. All-electron *GW* calculation of the electronic structure in light-element-doped TiO_2
    The 11th General Conference of the Asian Consortium on Computational Materials Science（ACCMS-11）
    Yokohama, Japan（2025.6.1-3）No.I-56（Invited）
    Ryoji Sahara, Takashi Ishikawa, Kaoru Ohno, Kyosuke Ueda and Takayuki Narushima

29. Thermodynamic database comparison between first-principles calculations and neural network potential
    The 11th General Conference of the Asian Consortium on Computational Materials Science（ACCMS-11）
    Yokohama, Japan（2025.6.1-3）No.I-62（Invited）
    Arkapol Saengdeejin, Ryoji Sahara, Yoshiyuki Kawazoe, Kazuyuki Higashino, Hiori Kino and Toyohiro Chikyow

30. The effect of the MOF framework on electronic and structural properties of the encapsulated guest species
    The 11th General Conference of the Asian Consortium on Computational Materials Science（ACCMS-11）
    Yokohama, Japan（2025.6.1-3）No.I-71（Invited）
    Rodion V. Belosludov

31. Near-infrared mechanoluminescence of ZnO co-doped with Li and Nd
    The 11th General Conference of the Asian Consortium on Computational Materials Science（ACCMS-11）
    Yokohama, Japan（2025.6.1-3）No.O-3（Oral）
    Tomoki Uchiyama, A. Sakatani, R. Omori, K. Otonari, X. G. Zheng and C. N. Xu

32. Controlling NO_2 adsorption on defective graphene through strain: A DFT study
    The 11th General Conference of the Asian Consortium on Computational Materials Science（ACCMS-11）
    Yokohama, Japan（2025.6.1-3）No.P-15（Oral（Short））
    Meng Yin, Ying Chen, Hideo Miura and Ken Suzuki

33. Identifying Materials Genes Describing Catalytic CO2 Hydrogenation: an AI Approach with Theoretical and Experimental Data
    2025 International IRCCS-ILR-IRTG Symposium on “Cutting-Edge Synthesis and Functional Materials”
    Nagoya University, Nagoya, Japan（2025.6.11-12）（Poster）
    Ray Miyazaki, Kendra Belthle, Harun Tüysüz, Lucas Foppa and Matthias Scheffler

34. Quantum mechanical molecular dynamics modeling: Evolution of tribo-interfaces and emergence of superlubricity
    NEMD2025
    Osaka, Japan（2025.6.11-13）（Keynote）
    Takuya Kuwahara

35. Understanding the impact of Si, Ti, and Ge doping on the voltage profile of $LiNi_{0.5}Mn_{1.5}O_4$ cathodes for lithium-ion batteries
    EM-NANO 2025, The 10th International Symposium on Organic and Inorganic Electronic Materials and Related Nanotechnologies
    Fukui, Japan（2025.6.11-14）No.6-05（Oral）
    Tien Quang Nguyen, Shunsuke Narumi, Michihisa Koyama and Nobuyuki Zettsu

36. Molecular Insight into Adsorption and Conversion at the Liquid/Solid-Oxide Interface
    13th Triennial Congress of the World Association of Theoretical and Computational Chemists（WATOC 2025）
    Oslo, Norway（2025.6.22-27）No.681（Invited）
    Akira Nakayama

37. Non-Markovian proton/hydroxide ion transfer dynamics at the water/CeO_2 interface
    13th Triennial Congress of the World Association of Theoretical and Computational Chemists（WATOC 2025）
    Oslo, Norway（2025.6.22-27）No.709（Poster）
    Tatsushi Ikeda and Akira Nakayama

38. Exploring the free energy landscape of alkane C-C bond cleavage
    13th Triennial Congress of the World Association of Theoretical and Computational Chemists（WATOC 2025）
    Oslo, Norway（2025.6.22-27）No.764（Poster）
    Kenshin Takei, Tatsushi Ikeda, Koki Muraoka and Akira Nakayama

39. Influence of Vibronic Interactions on Charge Transfer Excitons in Nonfullerene Organic Photovoltaics
    The 42nd International Conference of Photopolymer Science and Technology（ICPST-42）
    Himeji City, Hyogo, Japan（2025.6.24-27）No.A11-08（Invited）
    Azusa Muraoka

40. Neural quantum states and many-variable variational Monte Carlo simulations
    Open software for neural wavefunctions
    Lausanne, Switzerland（2025.7.2-4）（Invited）
    Yusuke Nomura

41. Ab initio modelling of unconventional superconductors
    NCTS Physics 1-day CMMP Workshop on Ab Initio Approaches to Novel Properties of High Temperature Superconductors
    National Center for Theoretical Sciences（NCTS）, Taipei, Taiwan（2025.7.9）（Keynote）
    Ryotaro Arita

42. Develop a Closed-Loop Framework for AI Materials Lab
    Seminar of Suzhou University of Science and Technology
    Suzhou, China（2025.7.12）（Invited）
    Hao Li

43. Thermodynamic stability and defect trapping activity in Lead-free halide perovskites
    International Symposium on Solar Energy 2025（ISSE 2025）
    Kyushu University, Japan（2025.7.23-24）（Oral）
    Qing Wang, Ami Hiratsuka, Shota Kawachino and Satoshi Iikubo

44. Introduction to Digital Materials: A Digital Platform Driven Closed-Loop Framework for AI+Materials
    iCANX Talks
    Online（2025.7.25）（Invited）
    Hao Li

45. Tracking Diamond Tool Wear in Iron Machining with Machine Learning Simulation Study
    50th Vietnam Conference on Theoretical Physics（VCTP-50）
    Dalat city, Vietnam（2025.8.4-7）No.P.7（Poster）
    Nguyen Trinh Bao Anh, Enriquez John Isaac Guinto, Halim Harry Handoko, Ogiwara Hiroyuki, Yamasaki Takahiro, Michiuchi Masato, Oguchi Tamio and Morikawa Yoshitada

46. Decoding Fictive Temperature in Simulated Silica Glass: Implications for Optical Material Design
    5th International Workshop on Challenges of Atomistic Simulations of Glasses and Amorphous Materials
    Yokohama, Japan（2025.8.6-8）No.8（Poster）
    Shunsuke Hiiro, Liping Huang and Madoka Ono

47. Molecular Dynamics–Based Structural Interpretation of Alkali Borosilicate Glass for Understanding Experimental Results
    5th International Workshop on Challenges of Atomistic Simulations of Glasses and Amorphous Materials
    Yokohama, Japan（2025.8.6-8）No.9（Poster）
    Shunsuke Hiiro, Liping Huang and Madoka Ono

48. Decoding Fictive Temperature in Simulated Silica Glass: Implications for Optical Material Design
    The 17th International Conference on the Physics of Non-Crystalline Solids（PNCS17）
    Tsukuba, Japan（2025.8.10-13）No.P41（Poster）
    Shunsuke Hiiro, Liping Huang and Madoka Ono

49. Molecular Dynamics–Based Structural Interpretation of Alkali Borosilicate Glass for Understanding Experimental Results
    The 17th International Conference on the Physics of Non-Crystalline Solids（PNCS17）
    Tsukuba, Japan（2025.8.10-13）No.P45（Poster）
    Kei Chiba, Shunsuke Hiiro, Junjie Zhao and Madoka Ono

50. Molecular insight into the adsorption and conversion at the liquid/solid-oxide interface
    ACS Fall 2025 Digital Meeting, Development of Theoretical Methods, Algorithms and Applications to Relevant Chemical Problems
    Online（2025.8.17-21）No.4336136（Plenary）
    Akira Nakayama

51. First-principles analysis of in-plane anomalous Hall effect using symmetry-adapted Wannier Hamiltonians and cluster multipole decomposition
    PSI-K 2025
    Lausanne, Switzerland（2025.8.25-28）No.C8.32（Oral）
    Hiroto Saito and Takashi Koretsune

52. Materials Genes of CO_2 Hydrogenation on Supported Cobalt Catalysts: an AI Approach Integrating Theoretical and Experimental Data
    EuropaCat 2025 - 16th European Congress on Catalysis
    Trondheim, Norway（2025.8.31-9.5）No.481（Oral）
    Ray Miyazaki, Kendra S Belthle, Harun Tüysüz, Lucas Foppa and Matthias Scheffler

53. Flat Silicene and Beyond: Beryllium-Enhanced Stability and Electronic Characteristics
    22nd International Symposium on Organometallic Chemistry Directed Towards Organic Synthesis
    Kyoto, Japan（2025.9.1-5）No.PA-116（Poster）
    Masae Takahashi

54. Coarse-Grained Molecular Dynamics Simulation Analysis of the Effect of Heterogeneous Structures on the Wear Properties of Concentrated Polymer Brush
The Materials Science Student Workshop jointly organized by National Tsing Hua University and Tohoku University
Hsinchu, Taiwan（2025.9.3-4）
Y. Hara, Y. Ootani, C. Suzuki, Y. Su, S. Fukushima, N. Ozawa and M. Kubo

55. Introduction to Digital Materials: AI+Materials-Driven Closed-Loop Framework on Digital Platforms
CNNEM 2025
Changchun, China（2025.9.7）（Keynote）
Hao Li

56. Digital Materials-Driven Design of Surfaces and Interfaces: Intelligent Exploration from Catalysis to Energy
CNNEM 2025
Changchun, China（2025.9.7）（Keynote）
Hao Li

57. Introduction to Digital Materials: A Digital Platform Driven Closed-Loop Framework for AI+Materials
CNNEM 2025
Changchun, China（2025.9.7）（Keynote）
Hao Li

58. Introduction to Digital Materials: A Digital Platform Driven Closed-Loop Framework for AI+Materials
Seminar of Changchun Institute of Applied Chemistry, Chinese Academy of Sciences
Changchun, China（2025.9.8）（Invited）
Hao Li

59. MAPEAMENTO DA CURVA DE TRANSFORMAÇÃO DE FASE POR RESFRIAMENTO CONTÍNUO DE UM AÇO LAMINADO A FRIO NO SIMULADOR TERMOMECÂNICO GLEEBLE
ABM WEEK 9ª edição - 2025, 78º Congresso Anual da ABM – Internacional
São Paulo, Brazil（2025.9.9-11）（Oral）
João Pedro Gomes Coelho, Bruno Fernandes Mudesto, Celso Luiz Moraes Alves and Daniel Alexandre da Costa Ximenes

60. First-principles phase field method of microstructures in high-temperature alloys
E-MRS 2025 Fall Meeting（European Materials Research Society）
Warsaw, Poland（2025.9.15-18）No.#00541（Invited）
Ryoji Sahara, Rohit Sanjay Dahule, Thi Nu Pham, Swastibrata Bhattacharyya, Riichi Kuwahara and Kaoru Ohno

61. DFT and Experimental Insights into Strain-Controlled Enhancement of Sensing Performance in Graphene Gas Sensors
    SSDM2025（2025 International Conference on Solid State Devices and Materials）
    Yokohama, Japan（2025.9.15-18）No.K-6-03（Oral）
    Meng Yin, Xiangyu Qiao, Yunsong Tang, Ying Chen, Hideo Miura and Ken Suzuki

62. Artificial Intelligence Approaches Toward Catalytic Chemistry
    International Workshop on First-principles and Artificial-Intelligence Methods for Materials
    Juist, Island in the North Sea, Germany（2025.9.15-19）（Keynote）
    Ray Miyazaki

63. Introduction to Digital Materials: A Digital Platform Driven Closed-Loop Framework for AI+Materials
    Pujiang Innovation Forum 2025 - International Future Chemistry Forum
    Shanghai, China（2025.9.20-22）（Invited）
    Hao Li

64. Introduction to Digital Materials: A Digital Platform Driven Closed-Loop Framework for AI+Materials
    Seminar of Fudan University
    China（2025.9.21）（Invited）
    Hao Li

65. Chemistry in Space Probed via Raman Spectroscopy of Forsterite and Mass Spectrometry of Gas-Phase Mineral Clusters
    The 9th Asian and Oceanian Spectroscopy Conference（AOSC-2025）
    Bogmallo Beach Resort, Goa, INDIA（2025.9.21-25）（Invited）
    Masashi Arakawa

66. Exploration of Organic Solar Cell Materials via Machine Learning and Vibronic Interaction of Charge Separation Dynamics
    Optical Probe2025-The 15th International Conference on Optical Probes of Organic and Hybrid Semiconductors（OP2025）
    Fukuoka, Japan（2025.9.21-26）No.IN28（Invited）
    Azusa Muraoka

67. AI-driven Hydrogen Storage Material Data Platform
    Global IEA Meeting for Hydrogen Storage Materials,（Sept 2025）
    Online（2025.9.22）（Invited）
    Hao Li

68. Innovating Battery Cathode Materials with Modeling and Machine Learning: Insights from Simulation-Experiment Synergy
    9th Academic Conference on Natural Science for Young Scientists, Master and PhD Students from ASEAN countries（CASEAN - 9）
    Khanh Hoa Province, Vietnam（2025.9.28-10.1）No.B-04（Invited）
    Tien Quang Nguyen, Michihisa Koyama and Nobuyuki Zettsu

69. Exploring the Thermodynamic Stability of the High Entropy Ultra-High Temperature Ceramic Composition Space（Ti,Zr,Hf,Nb,Ta）C_{1-x}
    MS&T25
    Columbus, Ohio, USA（2025.9.28-10.1）（Invited）
    Theresa Davey and Ying Chen

70. Turing Scheme for Materials – An Intelligent Digital Platform Powered by Ultra-Large-Scale Exp + Comput Data
    The 3rd World Materials Conference, the 9th World Materials Summit, and the 26th IUMRS-ICA（3rd WMC, 9th WMS & IUMRS-ICA2025）
    Guilin, Guangxi, China（2025.10.14-17）（Keynote）
    Hao Li

71. Data-Driven Closed-Loop Frameworks for Energy Materials Design
    The 3rd World Materials Conference, the 9th World Materials Summit, and the 26th IUMRS-ICA（3rd WMC, 9th WMS & IUMRS-ICA2025）
    Guilin, Guangxi, China（2025.10.14-17）（Invited）
    Xue Jia

72. A facile synthesis of peropyrene derivatives
    15th Japan-China Joint Symposium on Conduction and Photoconduction in Organic Solids and Related Phenomena
    Worldhotel Grand Dushulake Suzhou, China（2025.10.24-27）（Invited）
    Kazuo Takimiya

73. Origin for the Colossal Permittivity in doped TiO_2
    TACT2025 International Thin Films Conference
    Taipei, Taiwan（2025.10.26-29）No.B-I-475（Invited）
    Van An Dinh, Yujiro Hashimoto, Koji Kimura, Taro Kuwano, Dung Ngoc Dinh, Ryoji Asahi, Koichi Hayashi, Hiroki Taniguchi and Yoshitada Morikawa

74. Employing Machine Learning Molecular Dynamics to Probe Diamond Tool Degradation in Iron Cutting
    The 26th Asian Workshop on First-Principles Electronic Structure Calculations（ASIAN-26）
    Tsukuba International Congress Center, Tsukuba, Japan（2025.10.27-29）
    No.47（Poster）
    Nguyen Trinh Bao Anh, Enriquez John Isaac Guinto, Halim Harry Handoko, Ogiwara Hiroyuki, Yamasaki Takahiro, Michiuchi Masato, Oguchi Tamio and Morikawa Yoshitada

75. Theoretical Insight into Alkane Hydrogenolysis Based on Free Energy Landscape
    The 26th Asian Workshop on First-Principles Electronic Structure Calculations（ASIAN-26）
    Tsukuba International Congress Center, Tsukuba, Japan（2025.10.27-29）
    No.173（Poster）
    Kenshin Takei

76. Assessing p-Type Dopability in Oxygen 2p-Dominated Electronic States
    The 26th Asian Workshop on First-Principles Electronic Structure Calculations（ASIAN-26）
    Tsukuba International Congress Center, Tsukuba, Japan（2025.10.27-29）
    No.182（Poster）
    Vu Thi Ngoc Huyen and Yu Kumagai

77. High strength and high ductility of ultrafine grained ultralfine grained Titanium alloy through high density electric current
    The 9th International Conference on Nanomaterials by Severe Plastic Deformation（NanoSPD9）
    Beijing, China（2025.10.31-11.4）（Invited）
    Yongpeng Tang

78. Introduction to Digital Materials: A Digital Platform Driven Closed-Loop Framework for AI+Materials
    1st International Conference on Molecular Simulation & Intelligent Chemical Engineering
    Beijing, China（2025.11.1）（Plenary）
    Hao Li

79. Molecular simulation of surfaces and interfaces using neural network potentials
    The 9th Thailand International Nanotechnology Conference（NanoThailand 2025）
    Bangkok, Thailand（2025.11.3-5）No.S08-K-01（Keynote）
    Akira Nakayama

80. Vibronic Pathway Engineering for Efficient Exciton Separation in High-Efficiency Nonfullerene OSCs
    EU-Japan in HPC Hanami Project, Materials Science from First Principles: Materials Scientist Toolbox
    Sorbonne University, Paris, France（2025.11.3-7）（keynote）
    Azusa Muraoka

81. Three-dimensional Finite Element Analysis on Reconstructed Microstructures of MoSiBTiC Alloy Using SliceGAN
    International symposium MSSp2025, Materials Science and Spintronics for Sustainable Futures from Tohoku 2025
    Sendai, Japan（2025.11.4-7）No.GP-MS-3-3（Oral）
    Hiromu Matsuura, Junfeng Du, Chihana Kudo and Kyosuke Yoshimi

82. Coarse-Grained Molecular Dynamics Study of Cross-Linked Concentrated Polymer Brushes for Improved Wear Resistance
    International symposium MSSp2025, Materials Science and Spintronics for Sustainable Futures from Tohoku 2025
    Sendai, Japan（2025.11.4-7）No.MS-1（Poster）
    Y. Hara, Y. Ootani, C. Suzuki, Y. Su, S. Fukushima, N. Ozawa and M. Kubo

83. First-principles Study of Strain-Controlled Band Alignment in Chemiresistive Materials for Gas Sensing Enhancement
    International symposium MSSp2025, Materials Science and Spintronics for Sustainable Futures from Tohoku 2025
    Sendai, Japan（2025.11.4-7）No.MS-12（Poster）
    M. Yin, Y. Chen, H. Miura, A. Guntner and K. Suzuki

84. Unraveling the Complexity of Divalent Hydride Electrolytes in Solid-State Batteries via a Data-Driven Framework with Large Language Model
    International symposium MSSp2025, Materials Science and Spintronics for Sustainable Futures from Tohoku 2025
    Sendai, Japan（2025.11.4-7）No.MS-21（Poster）
    Qian Wang

85. Atomic configuration of the Nd-doped Σ13 grain boundary in MgO
    International symposium MSSp2025, Materials Science and Spintronics for Sustainable Futures from Tohoku 2025
    Sendai, Japan（2025.11.4-7）No.MS-43（Poster）
    Qian Chen, Mitsuhiro Saito, Kazuaki Kawahara, Kazutoshi Inoue, Atsutomo Nakamura and Yuichi Ikuhara

86. Digital Materials Ecosystem: A Digital Platform Driven Closed-Loop Framework for AI+Materials
    9th Forum of Materials Genome Engineering（ForMGE）
    Xi’an, China（2025.11.9）（Plenary）
    Hao Li

87. Introduction to Digital Materials: A Digital Platform Driven Closed-Loop Framework for AI+Materials
    Seminar of Xi’an Jiaotong University
    Xi’an, China（2025.11.9）（Invited）
    Hao Li

88. Effect of Ligand Structure on Interfacial Behavior at the Nanoscale Interface between Surface-Modified Ag and Curing Agent
    22nd International Conference on Flow Dynamics（ICFD2025）
    Sendai, Miyagi, Japan（2025.11.10-13）No.OS27-46（Poster）
    Yoichiro Kurosawa, Takamasa Saito, Yohei Okada, Manabu Inutsuka, Chiharu Tokoro, Eita Shoji, Momoji Kubo and Masaki Kubo

89. From Equations to Superconductors: Matter Under Pressure
    Presidential Lecture, Simons Foundation
    New York, USA（2025.11.12）（Invited）
    Ryotaro Arita

90. Data-Driven Closed-Loop Frameworks for Energy Materials Design
    9th International Forum of Materials Genome Engineering
    Xi’an, Shaanxi, China（2025.11.19-23）（Oral）
    Xue Jia

91. Can atomic-scale tribochemistry explain macroscale friction and wear?
    France-Japan Forum 2025（JSPS–JST）
    Lyon, France（2025.11.24-26）（Invited）
    Takuya Kuwahara

92. Exploring Transition Metal High Entropy Alloys from First-principles and Machine Learning
    ACCMS Webinar
    Online（2025.11.25）No.38（Invited）
    Ying Chen

93. Digital Materials Ecosystem: A Digital Platform Driven Closed-Loop Framework for AI+Materials
    Training Workshop, University of Shanghai for Science and Technology
    Online（2025.11.25）（Invited）
    Hao Li

94. First-Principles Investigation of Defect Properties of ZnO-Based Mechanoluminescent Materials
ML-5（Mechanoluminescence and Novel Structural Health Diagnosis）
Xiamen, China（2025.11.28-30）
Guangfa Yang, K. Otonari, R. Omori, M. Kimura, T. Uchiyama, Y. Chen and C. N. Xu

95. Noble Mechanism of Colossal Permittivity in Nb-doped TiO_2
2025 MRS Fall Meeting & Exhibit
Boston, Massachusetts, USA（2025.11.30-12.5）No.EL05.09.01（Oral）
Van An Dinh, Yujiro Hashimoto, Koji Kimura, Taro Kuwano, Dung Ngoc Dinh, Ryoji Asahi, Koichi Hayashi, Hiroki Taniguchi and Yoshitada Morikawa

96. Automated 2D Finite Element Analysis on Synthesized Microstructures of MoSiBTiC Alloy Using Generative AI
2025 MRS Fall Meeting & Exhibit
Boston, Massachusetts, USA（2025.11.30-12.5）No.MT03.09.14（Oral）
Hiromu Matsuura, Junfeng Du, Chihana Kudo, Takahiro Kaneko and Kyosuke Yoshimi

97. Quantum many-body solver using neural networks and its applications to strongly correlated electron systems
Fermionic Neural Quantum States: Recent Progress
Paris, France（2025.12.1-2）（Invited）
Yusuke Nomura

98. A Molecular Dynamics Simulation Study on Interfacial Slip and Rheology of Immiscible Polymer Blends
The 21st Asian Workshop on Polymer Processing（AWPP2025）
Kanazawa, Japan（2025.12.1-4）No.P0034（Poster）
Takeshi Sato, Kenji Yoshimoto and Kentaro Taki

99. Computational Chemistry and Machine-learning Approaches to Multi-element Materials for Energy and Environmental Applications
Cambodian Chemical Society International Symposium（CCSIS2025）
Phnom Penh, Cambodia（2025.12.5-8）（Invited）
Michihisa Koyama

100. Improving the Precision of Materials Property Prediction via Self-Supervised Pretraining
The 14th International Conference on Advanced Materials and Devices（ICAMD2025）
BEXCO Convention Hall, Busan, Korea（2025.12.8-12）
No.PO-AC25-383（Poster）
Hinata Ota, Shin Kiyohara and Yu Kumagai

101. Exploration of novel high-dielectric materials using deep kernel learning
The 14th International Conference on Advanced Materials and Devices（ICAMD2025）
BEXCO Convention Hall, Busan, Korea（2025.12.8-12）
No.PO-AC25-522（Poster）
Ruon Katsuragi, Shin Kiyohara and Yu Kumagai

102. First-principles study of Mg-ion diffusion in α-MnO_2
The 14th International Conference on Advanced Materials and Devices（ICAMD2025）
BEXCO Convention Hall, Busan, Korea（2025.12.8-12）
No.PO-AC25-658（Poster）
Haruki Shinohara, Shin Kiyohara and Yu Kumagai

103. Origin for the Colossal Permittivity in Nb doped rutile TiO_2: Flip-flop Motion of Molecular Polaron through Doped Nb
Materials Research Meeting 2025（MRM2025）
Yokohama, Japan（2025.12.8-13）No.A1-O201-01（Invited）
Van An Dinh, Yujiro Hashimoto, Koji Kimura, Taro Kuwano, Dung Ngoc Dinh, Ryoji Asahi, Koichi Hayashi, Hiroki Taniguchi and Yoshitada Morikawa

104. Anharmonic Phonon Property Database Based on Brute-Force First-Principles Calculations
Materials Research Meeting 2025（MRM2025）
Yokohama, Japan（2025.12.8-13）No.A2-O302-09（Oral）
Masato Ohnishi

105. Highly Active Catalyst Layer Structure in Polymer Electrolyte Fuel Cell Cathode: Large-Scale Reactive Molecular Dynamics Study
Materials Research Meeting 2025（MRM2025）
Yokohama, Japan（2025.12.8-13）No.B1-O201-06（Oral）
Nobuki Ozawa, Kaito Mori, Tetsuya Nakamura and Momoji Kubo

106. Analysis of PhD Human Resource Development Trends in Computational Materials Science for “Fugaku” Utilization: Research Field Identification via Expert-Curated Keywords and LLM-Assisted Text Mining
Materials Research Meeting 2025（MRM2025）
Yokohama, Japan（2025.12.8-13）No.B1-O301-05（Oral）
Yayoi Terada

107. A Neural Network Interatomic Potential for the Ternary α-Fe–C–H System: Toward an Atomistic Understanding of the Hydrogen Embrittlement in Steel
Materials Research Meeting 2025（MRM2025）
Yokohama, Japan（2025.12.8-13）No.B2-O301-03（Oral）
Fan-Shun Meng, Kazuki Matsubara and Shigenobu Ogata

108. Diffusion Model with Adaptive Constraint Guidance for Inorganic Phase Generation
Materials Research Meeting 2025（MRM2025）
Yokohama, Japan（2025.12.8-13）No.B2-O302-02（Oral）
Auguste de Lambilly, Vladimir Baturin, Jean-Claude Crivello, Guillaume Lambard, David PorteHault, Florence d'Alché-Buc and Nataliya Sokolovska

109. *p*-Type Dopability in Oxides with Oxygen 2*p*-Dominated Valence Bands
Materials Research Meeting 2025（MRM2025）
Yokohama, Japan（2025.12.8-13）No.B3-O201-01（Oral）
Vu Thi Ngoc Huyen

110. Introduction to "Digital Materials": A Digital Platform Driven Closed Loop Framework for AI+Materials
AI Agent Focus Talk
Online（2025.12.10）（Invited）
Hao Li

111. Ordered Phases in Mixed Crystals: High-entropy Alloys and III-V Compounds
182nd Structural Materials Seminar: From fundamental understanding through atomistic simulations to hypersonic technology development
Tsukuba, Japan（2025.12.15）（Invited）
Hiroshi Mizuseki

112. Molecular insight into the adsorption and conversion at the liquid/solid-oxide interface
The International Chemical Congress of Pacific Basin Societies 2025
（Pacifichem 2025）
Honolulu, HI, USA（2025.12.15-20）（Invited）
Akira Nakayama

113. Effects of vibronic coupling on exciton dissociation in NFA-based organic solar cells
The International Chemical Congress of Pacific Basin Societies 2025
（Pacifichem 2025）
Honolulu, HI, USA（2025.12.15-20）（Oral）
Azusa Muraoka

114. Prediction of high JSC donor molecules in fullerene-type organic solar cells using machine learning
The International Chemical Congress of Pacific Basin Societies 2025
（Pacifichem 2025）
Honolulu, HI, USA（2025.12.15-20）（Oral）
Azusa Muraoka

115. Effect of Sliding Conditions on MoS_2 Film Formation Process by Neural Network Molecular Dynamics Simulation
The International Chemical Congress of Pacific Basin Societies 2025 (Pacifichem 2025)
Honolulu, HI, USA (2025.12.15-20) (Oral)
Chihiro Suzuki, Yukihi Hara, Yixin Su, Shogo Fukushima, Yusuke Ootani, Nobuki Ozawa and Momoji Kubo

116. Influence of ionomer/carbon ratio on electrode reaction activity in cathode catalyst layer of polymer electrolyte fuel cells: reactive molecular dynamics simulation
The International Chemical Congress of Pacific Basin Societies 2025 (Pacifichem 2025)
Honolulu, HI, USA (2025.12.15-20) (Oral)
K. Mori, T. Nakamura, Y. Su, S. Fukushima, Y. Ootani N. Ozawa and M. Kubo

117. Relationship between wear resistance and crosslinking position in concentrated polymer brushes using coarse-grained molecular dynamics
The International Chemical Congress of Pacific Basin Societies 2025 (Pacifichem 2025)
Honolulu, HI, USA (2025.12.15-20) (Oral)
Y. Hara, Y. Ootani, C. Suzuki, Y. Su, S. Fukushima, N. Ozawa and M. Kubo

118. Theoretical study of exciton dissociation processes in NTz-based non-fullerene organic solar cells
The International Chemical Congress of Pacific Basin Societies 2025 (Pacifichem 2025)
Honolulu, HI, USA (2025.12.15-20) No.Board 079 (Poster)
Haruka Araragi, Seihou Jinnai, Yutaka Ie and Azusa Muraoka

119. Machine learning discovery of non-fullerene acceptor materials for organic solar cells with a fixed donor molecule
The International Chemical Congress of Pacific Basin Societies 2025 (Pacifichem 2025)
Honolulu, HI, USA (2025.12.15-20) No.Board 087 (Poster)
Azusa Muraoka

120. Theoretical study on nitrogen triple bond cleavage and ammonia formation in nitrogen reduction reactions catalyzed by Li and Ca
The International Chemical Congress of Pacific Basin Societies 2025 (Pacifichem 2025)
Honolulu, HI, USA (2025.12.15-20) No.Board 090 (Poster)
Chinami Okamura, Koichi Yamashita and Azusa Muraoka

121. Impact of Br substitution on structural and defect properties of Sn/Ge double perovskite solar cell materials: a first-principles approach
The International Chemical Congress of Pacific Basin Societies 2025 （Pacifichem 2025）
Honolulu, HI, USA（2025.12.15-20）No.Board 121（Poster）
Mai Otake, Suzune Omori, Masanori Kaneko, Maurizia Palummo, Giacomo Giorgi, Koichi Yamashita and Azusa Muraoka

122. DFT study of electronic states and thermoelectric properties of n-type doped carbon nanotubes
The International Chemical Congress of Pacific Basin Societies 2025 （Pacifichem 2025）
Honolulu, HI, USA（2025.12.15-20）No.Board 268（Poster）
Miya Matsuzaki, Mina Shimamoto, Achmad Syarif Hidayat, Naoki Ueoka, Yutaka Matsuo and Azusa Muraoka

123. Vibronic Coupling for Efficient Exciton Separation in High-efficiency Nonfullerene Organic Solar Cell
16th Ewha-JWU-Ochanomizu Joint Symposium
Ochanomizu University, Japan（2025.12.21-23）（Plenary）
Azusa Muraoka

124. Analysis of band gap in perovskite using explainable ML with structural descriptors
16th Ewha-JWU-Ochanomizu Joint Symposium
Ochanomizu University, Japan（2025.12.21-23）
Saho Kobayashi-Kajikawa and Azusa Muraoka

125. First-Principles Study on the Electronic Structures of 2D and 2D/3D Hybrid Organic–Inorganic Perovskites
16th Ewha-JWU-Ochanomizu Joint Symposium
Ochanomizu University, Japan（2025.12.21-23）
Nao Muramatsu and Azusa Muraoka

126. Analysis of Structural Factors and Band Gaps in Lead-Based Layered Perovskites Using Machine Learning
16th Ewha-JWU-Ochanomizu Joint Symposium
Ochanomizu University, Japan（2025.12.21-23）
Akina Sato, Saho Kobayashi-Kajikawa and Azusa Muraoka

＜2026年＞

1. Digital Materials Ecosystem: A Digital Platform Driven Closed-Loop Framework for AI+Materials
Seminar of Nanjing Forestry University
Nanjing, China（2026.1.3）（Invited）
Hao Li

2. Data-Driven Closed-Loop Frameworks for Energy Materials Design
   2026 National Conference on Advanced Battery Materials and Energy Catalysis Materials
   Nanjing, Jiangsu, China（2026.1.3-5）（Invited）
   Xue Jia

3. Digital Materials Ecosystem: A Digital Platform Driven Closed-Loop Framework for AI+Materials
   2026 National Conference on Frontier Battery Materials and Energy Catalytic Materials
   Nanjing, China（2026.1.5）（Keynote）
   Hao Li

4. Material Digital Twin of Multi-element Materials for Catalysis and Electrochemical Energy Systems
   International Conference on Scientific Advances in Natural and Technological Sciences（SAiNTS - 2026）
   Bengaluru, India（2026.1.7-9）（Invited）
   Michihisa Koyama

5. AI and Big Data Empowering Solid Electrolyte Innovation: Development and Applications of the DigBat Database Platform
   The 5 th International Symposium on the Frontiers of Functional Materials Research: solid-state ionics and solid-state batteries
   Sendai, Japan（2026.2.4）（Invited）
   Qian Wang

6. Simulation–Experiment Synergy in Data-Driven Materials Design of Battery Cathode for Sustainable Energy
   UPLB-SU Workshop on Data-Driven Materials Design
   The University of the Philippines Los Baños, Laguna, Philippines（2026.2.10-11）
   T. Q. Nguyen, N. Zettsu and M. Koyama

7. Thermodynamic Database Development using Machine Learning Data
   4th International Conference on Materials Genome（ICMG - IV）ACCMS Theme Meeting
   SRM University-AP, Amaravati, Andhra Pradesh, India（2026.2.19-21）
   No.10（Invited）
   Arkapol Saengdeejing, Ryoji Sahara, Hiori Kino and Toyohiro Chikyow

8. Design of high temperature alloys by first-principles calculation and experiment
   4th International Conference on Materials Genome（ICMG - IV）ACCMS Theme Meeting
   SRM University-AP, Amaravati, Andhra Pradesh, India（2026.2.19-21）
   No.15（Invited）
   Ryoji Sahara, Prasenjit Ghosh, Kyosuke Ueda, Takayuki Narushima and Yoko Yamabe-Mitarai

9. Knowledge-driven screening of phase stability in high-entropy alloys: The effect of valence electron concentration on crystal structures
   4th International Conference on Materials Genome（ICMG - IV）ACCMS Theme Meeting
   SRM University-AP, Amaravati, Andhra Pradesh, India（2026.2.19-21）
   No.16（Invited）
   Hiroshi Mizuseki

10. Time-dependent GW molecular dynamics: A new possible paradigm for accurately traversing the excited-state dynamical landscape
    4th International Conference on Materials Genome（ICMG - IV）ACCMS Theme Meeting
    SRM University-AP, Amaravati, Andhra Pradesh, India（2026.2.19-21）
    No.17（Invited）
    Aaditya Manjanath, Ryoji Sahara, Kaoru Ohno and Yoshiyuki Kawazoe

11. Design and synthesis of high-mobility molecular semiconductor crystals
    The 3rd GP Chem International Symposium
    Sendai, Japan（2026.2.20-21）（Invited）
    Kazuo Takimiya

12. Time-dependent GW molecular dynamics – a new possible paradigm for an accurate description of dynamics of chemical reactions
    Materials Science and Metallurgical Engineering Special Seminar
    Indian Institute of Technology, Hyedabad（IITH）（2026.2.23）（Invited）
    Aaditya Manjanath, Ryoji Sahara, Kaoru Ohno and Yoshiyuki Kawazoe

13. A multi-scale modelling without empirical parameter to design structural materials
    Materials Science and Metallurgical Engineering Special Seminar
    Indian Institute of Technology, Hyedabad（IITH）（2026.2.23）（Invited）
    Ryoji Sahara, Arkapol Saengdeejing, Aaditya Manjanath and Rohit Sanjay Dahule

14. Thermodynamic Database Development using Machine Learning Data
    Materials Science and Metallurgical Engineering Special Seminar
    Indian Institute of Technology, Hyedabad（IITH）（2026.2.23）（Invited）
    Arkapol Saengdeejing, Ryoji Sahara, Hiori Kino and Toyohiro Chikyow

15. Data-driven discovery and mechanistic understanding of high-entropy battery materials
    International Workshop in Computational Nanomaterials Design
    National Institute of Technology, Akashi College, Hyogo, Japan（2026.3.2）
    No.5（Invited）
    Tien Quang Nguyen

16. An OCTA Training Course at PCoMS with Professor Kawakatsu and Developers: Comparing the Effectiveness of Onsite vs. Online Hands-on Seminars
    International Workshop on Computational Soft-Matter（IWCSM）2026
    Sendai, Japan（2026.3.5-6）（Oral）
    Yayoi Terada

17. Playing with elements: Focus on High Entropy Alloys-- First-principles and Machine Learning
    The 28th CBMR Seminar, NIMS
    Tsukuba, Japan（2026.3.6）（Invited）
    Ying Chen

18. Chemical Effects on Defect Structure and Dynamics in Solids
    Joint Workshop of Sun Yat-Sen University, Macau University of Science and Technology and Tohoku University
    Shenzhen（2026.3.10）（Invited）
    Qian Chen

19. Digital Materials Ecosystem: A Digital Platform Driven Closed-Loop Framework for AI+Materials
    CNM Colloquium Series
    Argonne National Laboratory, Chicago, USA（2026.3.12）（Seminar Talk）
    Hao Li

20. Exploring Order-Disorder Relationships of the High Entropy Ultra-High Temperature Ceramic Composition Space（Ti,Zr,Hf,Nb,Ta）C_{1-x}
    TMS 2026 Annual Meeting & Exhibition（TMS2026）
    San Diego, CA, USA（2026.3.15-19）（Invited）
    Theresa Davey and Ying Chen

21. Neural Network Interatomic Potentials for Simulating Dislocation Plasticity in Ceramics at the Atomic Scale
    TMS 2026 Annual Meeting & Exhibition（TMS2026）
    San Diego, CA, USA（2026.3.15-19）No.D-5（Poster）
    Shihao Zhang and Shigenobu Ogata

22. Revisiting the ring-opening mechanisms of oxirane using time-dependent GW molecular dynamics
    APS Global Physics Summit
    Denver, CO, USA（2026.3.15-20）（Oral）
    Aaditya Manjanath, Ryoji Sahara, Yoshiyuki Kawazoe and Kaoru Ohno

23. First-Principles Phase-Field Prediction of the Ni-Al Alloy Microstructures at Room Temperature
    APS Global Physics Summit
    Denver, CO, USA（2026.3.15-20）（Oral）
    Rohit Dahule, Aditya Gollapalli, Abhishek Kr. Singh, Arkapol Saengdeejing, Toyohiro Chikyow, Ryoji Sahara and Kaoru Ohno

Ⅳ．予稿集

＜ Proceeding　2025年＞

1. 大規模言語モデル支援による博士人材育成動向調査手法の迅速化－計算物質科学分野のキーワード抽出評価－
   工学教育研究講演会講演論文集
   第73回年次大会（2025年度）(2025) pp.82-83
   寺田弥生
   https://doi.org/10.20549/jseeja.2025.0_82

＜2024年＞

1. 真空層モデルを用いた pure ZrO_2の対応粒界に関する第一原理計算
   2024年度エンジニアリングセラミックス若手セミナー
   静岡県熱海市 ハートピア熱海（2024.8.29-30）(Oral)
   南大地、杉山弘輝、松井和己、多々見純一

＜2025年＞

1. Li および Ca を触媒とした窒素還元反応における窒素三重結合切断過程とアンモニア生成の理論的研究
   2025年第72回応用物理学会春季学術講演会
   東京理科大学 野田キャンパス＆オンライン（2025.3.14-17）
   No.14a-K209-7（Oral）
   岡村千奈美、村岡梓、山下晃一

2. NTz 系非フラーレン型有機薄膜太陽電池における電荷分離過程
   2025年第72回応用物理学会春季学術講演会
   東京理科大学 野田キャンパス＆オンライン（2025.3.14-17）
   No.15a-K405-10（Oral）
   蘭暖佳、陣内青萌、家裕隆、村岡梓

3. フラーレン系有機薄膜太陽電池における高 J_{SC}ドナー分子設計のための LOOCV を用いた機械学習アプローチ
   2025年第72回応用物理学会春季学術講演会
   東京理科大学 野田キャンパス＆オンライン（2025.3.14-17）
   No.15a-K405-11（Oral）
   森下裕未、鑓水美里、金子正徳、村岡梓

4. 第一原理計算を用いた Sn/Ge ダブルペロブスカイト型太陽電池材料の欠陥構造と電子特性の理論解析
   2025年第72回応用物理学会春季学術講演会
   東京理科大学 野田キャンパス＆オンライン（2025.3.14-17）
   No.16p-K405-8（Oral）
   大竹真愛、大森鈴音、金子正徳、Giorgi Giacomo、山下晃一、村岡梓

5. カルバゾールユニットを導入した *N,N*− 架橋型トリアリールボランの合成と遅延蛍光特性の評価
   日本化学会 第105春季年会（2025）
   関西大学 千里山キャンパス（2025.3.26-29）
   No.[F]2201-2pm-02（Oral）
   坂井田奈菜、北本雄一、服部徹太郎

6. All-electron GW approach for light-element-doped anatase TiO_2
   <8th online virtual seminar> “TOMBO Seminar: Introduction, Examples, and Hands On 2025 March”
   Web（2025.3.28）（Invited）
   Ryoji Sahara

7. CALPHAD-type Thermodynamic Database using First-principles Calculations and Neural Network Potential
   ナノ学会第23回大会
   東京都立大学（2025.5.14-15）No.P-80（Poster）
   Saengdeejing Arkapol, Sahara Ryoji, Kawazoe Yoshiyuki, Higashino Kazuyuki, Kino Hiori and Chikyow Toyohiro

8. 分子動力学シミュレーションを用いた表面修飾 Ag／硬化剤界面の構造および相互作用の評価
   第62回日本伝熱シンポジウム /HTSJ 国際伝熱シンポジウム
   沖縄県宜野湾市沖縄コンベンションセンター（2025.5.14-17）
   No.BPA-49（Poster）
   黒沢陽一朗、斎藤高雅、岡田洋平、犬束学、所千晴、庄司衛太、久保百司、久保正樹

9. Data-driven approaches in materials science
   French-Japanese workshop on Open science
   Tokyo, Japan（2025.5.15）（Invited）
   J.-C. Crivello

10. First-principles database for anharmonic phonon properties
    第9回フォノンエンジニアリング研究会
    沖縄県宮古島（2025.5.18-19）（Oral）
    大西正人、塩見淳一郎

11. Screening new Entropy Stabilized Oxides by DFT calculations and active learning
    Material Science: Modeling & Design in Action
    Tsukuba（2025.5.21-22）（Plenary）
    S. Junier, C. Barreteau, C. Bajan, G. Lambard and J.-C. Crivello

12. 第一原理計算と実験によるマルチピエゾ体の開発と機能向上
    日本希土類学会：第41回希土類討論会
    倉敷市民会館（2025.5.22-23）No.1A-12（Oral）
    鈴木慶人、熊田舜士、王俊豪、内山智貴、鄭旭光、徐超男

13. 鉄加工におけるダイヤモンド工具の摩耗：機械学習分子動力学アプローチ
    トライボロジー会議 2025 春 東京
    国立オリンピック記念青少年総合センター（2025.5.26-28）No.A12（Oral）
    Bao-Anh Nguyen-Trinh, John Isaac G. Enriquez, Harry Handoko Halim, Hiroyuki Ogiwara, Takahiro Yamasaki, Masato Michiuchi, Tamio Oguchi and Yoshitada Morikawa

14. 粗視化分子動力学シミュレーションによる不均一構造ポリマーブラシの摩耗挙動の解析
    トライボロジー会議 2025 春 東京
    国立オリンピック記念青少年総合センター（2025.5.26-28）No.C37（Oral）
    原幸日、大谷優介、鈴木千尋、蘇怡心、福島省吾、尾澤伸樹、久保百司

15. Introduction of TOMBO: All-Electron *GW* Approach using TOMBO for Light Element Doped TiO_2
    TOMBO Workshop
    Yokohama, Japan（2025.5.31）（Invited）
    Ryoji Sahara

16. Mechanical-chemical coupling cyclic wear model of Ti influencing by nano-interlayer in contact with HAp
    日本材料学会第74期学術講演会
    日本大学工学部（2025.5.31-6.1）No.217（Oral）
    PhamDinhDat、大塚雄市、宮下幸雄

17. 粗視化分子動力学法による濃厚ポリマーブラシの耐摩耗性と架橋導入位置の関係の解析
    日本コンピュータ化学会2025年春季年会
    東京科学大学大岡山キャンパス（2025.6.5-6）No.2O05（Oral）
    原幸日、鈴木千尋、蘇怡心、福島省吾、大谷優介、尾澤伸樹、久保百司

18. 機械学習の量子多体問題への応用
    物理屋のための機械学習講義
    筑波大学東京キャンパス / オンライン（2025.6.20）（Invited）
    野村悠祐

19. Study on Mechanism of Indirect-Direct Transition in MoS_2 thin films using Wannier model
    OSAKA-SYMML Workshop
    大阪大学中之島センター（大阪）（2025.6.30-7.1）No.1）（Oral）
    平井駿佑、寺田伊吹、鈴木通人

20. Investigation of the electronic structure origin of the piezomagnetic effect in antiferromagnetic Mn_3Sn
    OSAKA-SYMML Workshop
    大阪大学中之島センター（大阪）（2025.6.30-7.1）No.2）（Oral）
    菊地宗一郎、柳有起、Vu Thi Ngoc Huyen、鈴木通人

21. Optical anisotropy and electronic states of the pleochronic material $Ca_3ReO_5Cl_2$
    OSAKA-SYMML Workshop
    大阪大学中之島センター（大阪）（2025.6.30-7.1）No.3）（Oral）
    月原拓海、鈴木通人

22. 計算・情報科学
    触媒学会 第36回キャタリシススクール
    東京大学（2025.7.8-10）No.5（Invited）
    宮崎玲

23. 自由エネルギー地形によるアルカン水素化分解反応メカニズムの理論的解明
    第14回 JACI/GSC シンポジウム
    一橋大学一橋講堂（一部ライブ配信有）（2025.7.15-16）No.A-75（Poster）
    竹井健真、池田龍志、村岡恒輝、中山哲

24. 酸化ジルコニウム / 水界面における微視的構造の解析
    第14回 JACI/GSC シンポジウム
    一橋大学一橋講堂（一部ライブ配信有）（2025.7.15-16）No.F-08（Poster）
    大石桃李、池田龍志、中山哲

25. 静電相互作用をあらわに考慮した機械学習力場の開発
    第27回理論化学討論会
    九州大学西新プラザ（2025.7.22-24）No.1L07（Oral）
    池田龍志、中山哲

26. CeO_2／メタノール界面における微視的構造の理論的解析
    第27回理論化学討論会
    九州大学西新プラザ（2025.7.22-24）No.P311（Poster）
    坂口智隼、池田龍志、中山哲

27. 高分子材料の摩耗・破壊の理解に向けた分子動力学シミュレーション
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東京（2025.8.22）(Invited)
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28. 大規模言語モデル支援による博士人材育成動向調査手法の迅速化 －計算物質科学分野のキーワード抽出評価－
第73回年次大会・工学教育研究講演会
京都大学桂キャンパス（2025.8.27-29）No.1E07（Oral）
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29. セル界面近傍の溶質偏析がすべり変形抵抗に与える影響に関する分子動力学解析
日本 Additive Manufacturing 学会 第1回講演大会
東京都立産業貿易センター浜松町館（2025.9.1-3）No.S5-6（Oral）
君塚肇、三津原晟弘

30. 機械学習ポテンシャルを用いた表面・界面の分子シミュレーション
日本化学会北海道支部・環境物質科学セミナー
北海道大学・北海道札幌市（2025.9.5）(Invited)
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31. Boron-containing π-conjugated molecules exhibiting thermally activated delayed fluorescence with long- and short-range charge-transfer characteristics
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山形大学米沢キャンパス（2025.9.6-7）No.07A2（Invited）
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32. 第一原理計算による MoS_2薄膜における間接・直接遷移の変化機構の研究
第86回応用物理学会秋季学術講演会
名城大学天白キャンパス / オンライン（2025.9.7-10）No.7a-P05-60（Poster）
平井駿佑、寺田伊吹、鈴木通人

33. 鉱物クラスターの気相反応と鉱物のラマン分光で探る惑星系形成領域・惑星大気での化学過程
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広島県広島市広島国際会議場（2025.9.8）No.3（Invited）
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34. APLICAÇÃO DE TERMODINÂMICA COMPUTACIONAL PARA MAPEAMENTOS DE EQUILÍBRIO E ANÁLISE DE SÓLIDOS FORMADOS A PARTIR DE PROCESSOS CORROSIVOS EM ÁGUAS SALINAS
    ABM WEEK 9ª edição - 2025, 23º Enemet - Encontro Nacional de Estudantes de Engenharia Metalúrgica, de Materiais e de Minas
    São Paulo, Brazil（2025.9.9-11）（Oral）
    Ana Giulia Mirabet Cusatis, Nathália Cristina Leôncio Neves, Celso Luiz Moraes Alves, Júlia Mendes Sales, Flavia Maciel F. Guedes and Tatiana das Chagas Almeida

35. ハイブリッド汎関数を用いた水溶液系の機械学習ポテンシャルの開発と輸送特性評価への応用
    第19回分子科学討論会
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    池田龍志、中山哲

36. 非フラーレン型有機薄膜太陽電池における NTz 系材料の積層構造と電荷輸送特性
    第19回分子科学討論会
    広島国際会議場（2025.9.9-12）No.1P041（Poster）
    蘭暖佳、陣内青萌、家裕隆、村岡梓

37. 第一原理計算による Br 置換 Sn/Ge ダブルペロブスカイト太陽電池の電子物性解析
    第19回分子科学討論会
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    大竹真愛、金子正徳、Palummo Maurizia、Giorgi Giacomo、山下晃一、村岡梓

38. 電気化学的アンモニア合成における Li および Ca 媒介機構の研究
    第19回分子科学討論会
    広島国際会議場（2025.9.9-12）No.2P079（Poster）
    岡村千奈美、山下晃一、村岡梓

39. 機械学習を用いた P3HT・PBDB-T・PM6・PTQ10ドナー分子に対応する非フラーレン型アクセプター材料の探索
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    小林佐保、小倉佳奈子、後藤明果莉、金子正徳、村岡梓

40. ホスフィン系・アミン系分子吸着による SWCNT の n 型ドーピングに関する電子状態計算
    第19回分子科学討論会
    広島国際会議場（2025.9.9-12）No.3P033（Poster）
    松崎美哉、島元美奈、Achmad Syarif Hidayat、上岡直樹、松尾豊、村岡梓

41. Data-driven Design of High-entropy Materials for Energy and Environmental Applications
化学工学会第56回秋季大会 HQ-11 Japan-Korea-Taiwan Joint Symposium on Chemical Engineering
芝浦工業大学豊洲キャンパス（2025.9.16-18）No.CK107（Invited）
Michihisa Koyama

42. 第一原理フェーズフィールド法および SQS 法による鉄リッチ FeSi 合金の理論研究
第49回日本磁気学会学術講演会、シンポジウム
「モータ駆動用ゼロ磁歪電磁鋼材料の研究動向」
愛媛大学城北キャンパス（2025.9.16-19）No.16pA-4（Invited）
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43. 第一原理計算による多色性物質 $Ca_3ReO_5Cl_2$における光学異方性と電子状態の研究
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広島大学東広島キャンパス（2025.9.16-19）No.16aPS-24（Oral）
月原拓海、寺田伊吹、鈴木通人

44. 第一原理計算による MoS_2薄膜における間接・直接遷移の変化機構の研究
日本物理学会第80回年次大会（2025年）
広島大学東広島キャンパス（2025.9.16-19）No.16pPS-101（Oral）
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45. 第一原理計算を用いたノンコリニア反強磁性体 NbMnP における非線形ホール効果に関する理論研究
日本物理学会第80回年次大会（2025年）
広島大学 東広島キャンパス（2025.9.16-19）No.17aPS-93（Oral）
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46. 表面を含む格子欠陥材料における機械学習を用いた材料探索手法の開発
日本物理学会第80回年次大会（2025年）
広島大学東広島キャンパス（2025.9.16-19）No.17aSK108-5（Oral）
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47. ノンコリニア反強磁性体 Mn_3Sn におけるピエゾ磁気効果と電子状態の研究
日本物理学会第80回年次大会（2025年）
広島大学 東広島キャンパス（2025.9.16-19）No.18aPS-23（Oral）
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48. Atomistic Insights into Diamond Tool Degradation in Iron Machining Using Machine Learning Molecular Dynamics Simulations
2025年度精密工学会秋季大会学術講演会
京都大学吉田キャンパス（2025.9.17-19）No.A34（Oral）
Nguyen Trinh Bao Anh、Enriquez John Isaac Guinto、Halim Harry Handoko、荻原寛之、山崎隆浩、道内真人、小口多美夫、森川良忠

49. 自由エネルギー地形計算に基づくアルカン水素化分解反応の理論的解析
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東北大学青葉山キャンパス 青葉山コモンズ（2025.9.17-19）No.1G27（Oral）
竹井健真、池田龍志、村岡恒輝、中山哲

50. 反応分子動力学シミュレーションを用いた固体高分子形燃料電池カソード触媒層の I/C 比がアイオノマー / 水ネットワークに与える影響の解析
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51. 固体高分子形燃料電池アノードの燃料欠乏状態において高酸素発生反応活性を示す IrO2系触媒構造の第一原理計算による検討
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尾澤伸樹、久保百司

52. 担持金触媒によるアルキルエーテルの C-O 結合シリル化の反応機構解析
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53. 第一原理計算によるアルカリ金属イオン添加 ZnO の力学特性と電子状態
日本セラミックス協会第38回秋季シンポジウム
群馬大学荒牧キャンパス（2025.9.17-19）No.3C23（Oral）
内山智貴、川名惣一朗、音成航希、大森令央奈、鄭旭光、徐超男

54. 第一原理マテリアルズ・インフォマティクスの進展とハイエントロピー合金への展開
日本金属学会2025年秋期（第177回）講演大会
北海道大学札幌キャンパス（2025.9.17-19）No.S3.19（Keynote）
水関博志、佐原亮二、本郷研太

55. CoReRu HCP ハイエントロピー合金の変形挙動と変形機構の解明
日本金属学会2025年秋期（第177回）講演大会
北海道大学札幌キャンパス（2025.9.17-19）No.S3.24（Oral）
坂井勇介、梁少基、佐原亮二、御手洗容子

56. Nd 添加 MgOΣ13粒界における原子構造と電子状態の解明
日本金属学会2025年秋期（第177回）講演大会
北海道大学札幌キャンパス（2025.9.17-19）No.S4.22（Oral）
陳茜、井上和俊、斎藤光浩、川原一晃、中村篤智、幾原雄一

57. Ni 基合金における固溶強化・積層欠陥強化の原子論的解析
日本金属学会2025年秋期（第177回）講演大会
北海道大学札幌キャンパス（2025.9.17-19）No.S8.10（Oral）
君塚肇、三津原晟弘

58. β 型 Ti-Nb 合金中の溶質濃度ゆらぎが塑性変形に及ぼす影響に関する原子論的解析
日本金属学会2025年秋期（第177回）講演大会
北海道大学札幌キャンパス（2025.9.17-19）No.S8.20（Oral）
三津原晟弘、君塚肇

59. 一族元素添加 ZnO の第一原理計算による力学特性の予測と応力発光機能
日本金属学会2025年秋期（第177回）講演大会
北海道大学札幌キャンパス（2025.9.17-19）No.82（Oral）
内山智貴、音成航希、大森令央奈、楊光発、鄭旭光、西堀英治、徐超男

60. 日本における計算物質科学の人材育成動向に関する調査研究 ― 大規模言語モデルを用いた分野判別による解析 II ―
日本金属学会2025年秋期（第177回）講演大会
北海道大学札幌キャンパス（2025.9.17-19）No.139（Oral）
寺田弥生

61. 生体用 Co-Cr-W-Ni 合金の機械的特性および積層欠陥エネルギーに及ぼす炭素・窒素添加の影響
日本金属学会2025年秋期（第177回）講演大会
北海道大学札幌キャンパス（2025.9.17-19）No.172（Oral）
和田知己、檜山快、佐原亮二、上田恭介、成島尚之

62. 第一原理計算と機械学習による Cantor-derived ハイエントロピー合金の展開（２）
日本金属学会2025年秋期（第177回）講演大会
北海道大学札幌キャンパス（2025.9.17-19）No.214（Oral）
陳迎、Tran Nguyen-Dung、李子墨、倪軍

63. 核の量子効果と空孔による捕獲効果を考慮したバナジウム中水素拡散の機械学習分子シミュレーション
日本金属学会2025年秋期（第177回）講演大会
北海道大学札幌キャンパス（2025.9.17-19）No.P63（Poster）
大芝颯太、三津原晟弘、君塚肇

64. α-MnO_2における Mg イオン拡散に関する第一原理計算
日本金属学会2025年秋期（第177回）講演大会
北海道大学札幌キャンパス（2025.9.17-19）No.P181（Poster）
篠原遥紀、清原慎、熊谷悠

65. 自己教師あり事前学習を活用した物性予測の高精度化
日本金属学会2025年秋期（第177回）講演大会
北海道大学札幌キャンパス（2025.9.17-19）No.P243（Poster）
太田陽向、清原慎、熊谷悠

66. 深層カーネル学習を用いた新規高誘電材料の探索
日本金属学会2025年秋期（第177回）講演大会
北海道大学札幌キャンパス（2025.9.17-19）No.P245（Poster）
葛城瑠音、清原慎、熊谷悠

67. 9元高エントロピー合金における機械学習力場の構築と局所構造の解析
日本金属学会2025年秋期（第177回）講演大会
北海道大学札幌キャンパス（2025.9.17-19）No.P248（Poster）
原幸佑、加藤日向、大戸達彦、君塚肇

68. TiZr-Multi Principal Element 合金の組織と力学特性に対する添加元素の効果
日本金属学会2025年秋期（第177回）講演大会
北海道大学札幌キャンパス（2025.9.17-19）No.P349（Poster）
関根佑樹、吉野哲生、佐原亮二、御手洗容子

69. Matlantis が拓く計算材料科学の新展開～多元素材料の実在系構造と機能～
Matlantis User Conference 2025
東京コンファレンスセンター・品川（2025.10.8）（Invited）
古山通久

70. 濃厚ポリマーブラシの高耐摩耗化に向けた粗視化分子動力学シミュレーション解析
トライボロジー会議 2025 秋 函館
函館アリーナ（2025.10.8-10）No.G34（Oral）
原幸日、大谷優介、鈴木千尋、蘇怡心、福島省吾、尾澤伸樹、久保百司

71. ニューラルネットワーク分子動力学法による摩擦環境が MoS_2結晶化プロセスに及ぼす影響の解析
トライボロジー会議 2025 秋 函館
函館アリーナ（2025.10.8-10）No.G37（Oral）
鈴木千尋、原幸日、蘇怡心、福島省吾、大谷優介、尾澤伸樹、久保百司

72. Machine Learning Molecular Dynamics Insights into Carbon Detachment from Diamond Tools in Iron Cutting
2025年日本表面真空学会学術講演会
つくば国際会議場（2025.10.20-22）No.2F03（Oral）
Bao Anh Nguyen Trinh, John Isaac Guinto Enriquez, Harry Handoko Halim, Hiroyuki Ogiwara, Takahiro Yamasaki, Masato Michiuchi, Tamio Oguchi and Yoshitada Morikawa

73. TOMBO-TD*GW* 法による電子励起状態経由 DNA 内原子組み替え過程追跡
第12回「富岳」を中核とする HPCI システム利用研究課題成果報告会
THE GRAND HALL（品川）＆オンライン（2025.10.23-24）(Poster)
Yoshiyuki Kawazoe, Kaoru Ohno, Hiroshi Mizuseki, Ryoji Sahara,
Aaditya Manjanath and Vannajan Sanghiran Lee

74. Modeling heterogeneous catalysis by AI that integrates experimental and theoretical data
第55回石油・石油化学討論会
福島県郡山市（2025.10.30-31）No.2A09（Invited）
Ray Miyazaki

75. Dopant Screening for Interfacial Energy Control of $(Ni,Co)_2Si$ Precipitates in Cu-Ni-Co-Si Alloys: A First-Principles Study
日本銅学会第65回講演大会
兵庫県姫路市（2025.10.31-11.2）No.7（Oral）
Eun-Ae Choi、Seung Zeon Han、加藤秀実、千星聡

76. 実空間と波数空間から見る微視的物性機構の研究
磁性理論ミーティング（主催：産総研第一原理材料設計研究チーム）
オンライン（2025.11.4）(Invited)
鈴木通人

77. 非相溶高分子ブレンドの界面すべりとレオロジー：分子動力学法による検討
第13回ソフトマター研究会
京都大学益川ホール（2025.11.4-6）No.P2-08（Poster）
佐藤健

78. リチウム媒介窒素還元反応における ESM-RISM 計算による溶媒和ポテンシャルの解析
日本コンピュータ化学会2025年秋季年会
岐阜市文化センター（2025.11.7-9）No.1P09（Poster）
風野由衣、金子正徳、山下晃一、村岡梓

79. スマネン分子の反転運動に伴うエネルギー変化の理論的計算
日本コンピュータ化学会2025年秋季年会
岐阜市文化センター（2025.11.7-9）No.1P10（Poster）
八十田実々、馬場唯花、櫻井英博、村岡梓

80. アニオンチャネルを介したキノイドモノカチオンのスタッキング相互作用の理論計算
日本コンピュータ化学会2025年秋季年会
岐阜市文化センター（2025.11.7-9）No.1P11（Poster）
笠間栞、馬場唯花、櫻井英博、村岡梓

81. 2D、2D/3D ハイブリッド有機無機ペロブスカイトの第一原理計算による電子構造解析
日本コンピュータ化学会2025年秋季年会
岐阜市文化センター（2025.11.7-9）No.2P10（Poster）
村松奈桜、Giacomo Giorgi、金子正徳、山下晃一、村岡梓

82. Analysis of Defect Structures at the Ferrite/Cementite Interface Using Density Functional Theory
第35回日本 MRS 年次大会
北九州国際会議場（2025.11.10-12）No.S-P10-018（Poster）
K. Kato and H. Raebiger

83. 第一原理計算で結晶粒界エネルギーを評価するための真空層モデル
日本機械学会 M&M2025材料力学カンファレンス
熊本県熊本市 熊本城ホール（2025.11.10-13）No.OS1405（Oral）
杉山弘輝、南大地、松井和己、レービガー ハンネス、多々見純一

84. 第一原理計算による磁気弾性定数に及ぼす元素置換効果の理論的検討
日本機械学会 M&M2025材料力学カンファレンス
熊本県熊本市 熊本城ホール（2025.11.10-13）No.OS1804（Oral）
早川聡、山崎貴大、福健太郎、Varadwaj Arpita、Foggiatto Alexandre、
小嗣真人

85. グラフェン・CNT ハイブリッド型ガスセンサーの開発と感度および選択性の改善
日本機械学会第16回マイクロ・ナノ工学シンポジウム
ライトキューブ宇都宮、栃木（2025.11.10-13）No.10P4-PN-67（Poster）
唐雲松、菅原一真、YIN MENG、鈴木研

86. データ駆動型の科学におけるサイバー・フィジカル連携
令和7年度電気化学会北陸支部秋季大会（富山）
富山大学五福キャンパス（2025.11.13-14）No. 特別講演②（Invited）
古山通久

87. 自己教師あり事前学習による物性予測精度の向上
令和7年度 日本セラミックス協会 東北北海道支部 研究発表会
東北大学サイエンスキャンパスホール（2025.11.13-14）No.2A-01（Oral）
太田陽向、清原慎、熊谷悠

88. 深層カーネル学習を用いた新規高誘電材料の探索
令和7年度 日本セラミックス協会 東北北海道支部 研究発表会
東北大学サイエンスキャンパスホール（2025.11.13-14）No.2A-06（Oral）
葛城瑠音、清原慎、熊谷悠

89. 第一原理計算による α-MnO2中の Mg イオン拡散におけるドーピング効果の解明
令和7年度 日本セラミックス協会 東北北海道支部 研究発表会
東北大学サイエンスキャンパスホール（2025.11.13-14）No.2A-09（Oral）
篠原遥紀、清原慎、熊谷悠

90. （Li,Na）NbO_3系マルチピエゾ体の発光・圧電特性に及ぼす希土類共添加の影響
令和7年度 日本セラミックス協会 東北北海道支部 研究発表会
東北大学サイエンスキャンパスホール（2025.11.13-14）No.P-13S（Poster）
鈴木慶人、大和田瑛士、内山智貴、鄭旭光、徐超男

91. DFT Calculations of Defect Properties in ZnO
令和7年度 日本セラミックス協会 東北北海道支部 研究発表会
東北大学サイエンスキャンパスホール（2025.11.13-14）No.P-34S（Poster）
楊光発、音成航希、大森令央奈、内山智貴、鄭旭光、徐超男

92. 希土類添加（Li,Na）NbO_3系マルチピエゾ体の発光・圧電特性
令和7年度 日本セラミックス協会 東北北海道支部 研究発表会
東北大学サイエンスキャンパスホール（2025.11.13-14）No.P-45S（Poster）
大和田瑛士、鈴木慶人、内山智貴、鄭旭光、徐超男

93. 振動自由度の抑制による分子動力学モデルの新解釈
令和7年度 日本セラミックス協会 東北北海道支部 研究発表会
東北大学サイエンスキャンパスホール（2025.11.13-14）No.P-57S（Poster）
千葉渓、日色駿介、Junjie Zhao、小野円佳

94. 機械学習分子シミュレーションによる核の量子効果と空孔による捕獲効果を考慮したバナジウム中水素拡散係数の定量評価
第35回材料フォーラム TOKAI
名古屋大学（2025.11.21）No.M21（Poster）
大芝颯太、三津原晟弘、君塚肇

95. 長距離相互作用と整合する機械学習力場の開発
レア・イベントの計算科学 第8回ワークショップ
鳥取県立生涯学習センター（2025.11.23）（Invited）
池田龍志

96. CeO_2メタノール界面系における微視的構造の理論的解析
第39回分子シミュレーション討論会
くにびきメッセ・島根県松江市（2025.11.24-26）No.204P（Poster）
坂口智隼、池田龍志、中山哲

97. グランドカノニカルモンテカルロ法における挿入削除バイアス法の開発と機械学習ポテンシャルへの応用
第39回分子シミュレーション討論会
くにびきメッセ・島根県松江市（2025.11.24-26）No.239P（Poster）
池田龍志、中山哲

98. 第一原理計算と機械学習ポテンシャルによる合金状態図予測
マグネティックス / リニアドライブ合同研究会
長崎大学（2025.12.1-2）No.MAG-25-121（Oral）
佐原亮二、Saengdeejing Arkapol、木野日織、川添良幸、東野和幸、知京豊裕

＜2026年＞

1. 単結晶8YSZ 表面近傍の力学特性に及ぼす真空高温還元処理で生成した酸素空孔の影響
2026年年会 公益社団法人日本セラミックス協会
横浜国立大学 常盤台キャンパス（2026.3.4-6）No.1P139（Poster）
馬場流、多々見純一、大司達樹、飯島志行、高橋拓実、中野裕美

2. アルミニウム合金の時効析出過程の原子論：GP ゾーンの形成機構と力学的効果
「結晶欠陥と結晶塑性」研究会
北見工業大学（2026.3.5-6）
君塚肇

3. 原子・分子系のグランドカノニカルモンテカルロシミュレーション理論
凝縮系の理論化学
那覇文化芸術劇場なはーと・沖縄県那覇市（2026.3.11-12）（Invited）
池田龍志、中山哲

4. Hybrid Sampling Machine-Learning Potentials for Accurate Hydrogen Adsorption in MOF-303
日本金属学会2026年春期（第178回）講演大会
千葉工業大学新習志野キャンパス（2026.3.11-13）No.85（Oral）
Kartik Sau Sau, Ikutaro Hamada, Tamio Ikeshoji, Yiming Lu, Susmita Roy, Shohichi Furukawa, Linda Zhang, Hung Ba Tran, Takahiro Kondo, Hao Li and Shin-ichi Orimo

5. 計算材料科学分野の若手研究者支援のケーススタディ －計算物質科学人材育成コンソーシアムによるセミナー活動の現状と課題－
日本金属学会2026年春期（第178回）講演大会
千葉工業大学新習志野キャンパス（2026.3.11-13）No.128（Oral）
寺田弥生

6. First-Principles Study of $(Ni,Co)_2Si$ Precipitation Tuned by Interfacial Dopant Segregation in Cu-Ni-Co-Si Alloys
   日本金属学会2026年春期（第178回）講演大会
   千葉工業大学新習志野キャンパス（2026.3.11-13）No.170（Oral）
   Eun-Ae Choi, Byungki Ryu and Seung Zeon Han

7. 実験パラメータに依存しない階層計算技術による構造材料設計
   日本鉄鋼協会第191回春季講演大会
   千葉工業大学 新習志野キャンパス（2026.3.11-13）No.192（浅田賞受賞講演）
   佐原亮二

8. 光スイッチ分子を基盤とする動的溶媒の開発と錯体発光制御
   第9回分子ロボティクス年次大会
   東北大学 片平キャンパス（2026.3.12-13）No.P26（Poster）
   宮下元気（若手研究奨励賞）、高石慎也、坂本良太、豊田良順

9. 原子スケールフェーズフィールド法の開発
   2026年第73回応用物理学会春季学術講演会
   東京科学大学 大岡山キャンパス ＆オンライン（2026.3.15-18）
   No.15a-W9_323-5（Oral）
   益田快理、熊谷悠

10. Interplay of Defect Chemistry and Stability in Ge-Based Halide Perovskites
    2026年第73回応用物理学会春季学術講演会
    東京科学大学 大岡山キャンパス ＆オンライン（2026.3.15-18）
    No.16p-M_124-16（Oral）
    Qing Wang, Yusheng Li, Shota Kawachino, Qing Shen and Satoshi Iikubo

11. 自己教師あり事前学習を用いた物性予測精度の向上に関する研究
    2026年第73回応用物理学会春季学術講演会
    東京科学大学 大岡山キャンパス ＆オンライン（2026.3.15-18）
    No.17a-S2_204-1（Oral）
    清原慎、太田陽向、熊谷悠

12. 機械学習による HfO_2 の三次元ランダウ関数の構築とオンデマンド型フェーズフィールド法の開発
    2026年第73回応用物理学会春季学術講演会
    東京科学大学 大岡山キャンパス ＆オンライン（2026.3.15-18）
    No.18p-S2_204-3（Oral）
    田村友佑、益田快理、熊谷悠

13. Machine-Learning Interatomic Potential Molecular Dynamics Study for Understanding Diamond Tool Failure in Iron Cutting
    2026年度精密工学会春季大会学術講演会
    埼玉大学（2026.3.17-19）No.G57（Oral）
    Nguyen Trinh Bao Anh、Enriquez John Isaac Guinto、Halim Harry Handoko、荻原寛之、山崎隆浩、道内真人、小口多美夫、森川良忠

14. 表面修飾 Ag／エポキシ樹脂前駆体界面の親和性評価に関する分子動力学解析
    化学工学会第91年会
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Ⅴ．学位取得

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2. ラーベス相 $MgZn_2$に対する3d 遷移金属微量置換の効果に関する第一原理計算
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