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# 原著論文/著書リスト

## 原著論文/全て査読有(A206 以下が採録決定済/A212 以下が arXiv 済)

* A214; " Topological data analysis for revealing structural origin of density anomalies in silica glass",
(***)

A. Tirelli, K. Nakano,
arXiv: 2208.06378 (2022)

* A213; " High-$T_c$ superconductivity of clathrate $Y_3EuH_{24}$",
(クラスレート構造イットリウム・ユーロピウム水素化物の高温超伝導)

A. Ghaffar, P. Song, K. Nakano, K. Hongo, R. Maezono,
arXiv:2205.05906 (2022)

* A212; " Quantum phase diagram of high-pressure hydrogen",
(第一原理量子モンテカルロ法を利用した高圧水素の量子相図研究)

Lorenzo Monacelli, Michele Casula, Kosuke Nakano, Sandro Sorella, Francesco Mauri,
arXiv:2202.05740 (2022)

* A211; "High-$T_c$ ternary metal hydrides, $YKH_{12}$ and $LaKH_{12}$, discovered by machine learning",
(機械学習的探索で発見された高温超伝導 3 元水素化物)

P. Song, H. Zhufeng, P. Baptista de Castro, K. Nakano, K. Hongo, Y. Takano, R. Maezono,
arXiv:2103.00193 (2021)

* A210; "First Principles Calculations of Superconducting Critical Temperature of $ThCr_2Si_2$-Publisher Structure",
($ThCr_2Si_2$ 型化合物の超伝導転移温度に関するハイスループットスクリーニング)

G.S. Sinaga, K. Utimula, K. Nakano, K. Hongo, R. Maezono,
(in preparation for J. Phys. Chem. C (2022/IF= 3.7))
arxiv.org/abs/1911.10716

*A209; "Importance of vdW and long-range exchange interactions to DFT-predicted docking energies between plumbagin and cyclodextrins"

(シクロデキストリンのホストゲスト結合予見における電子相関)

T. Ichibha, O. Srihakulung, G. Chao, A. T. Hanindriyo, L. Lawtrakul, K. Hongo, R. Maezono,
arXiv:1904.02503(2019)

* A208; "Stable HCP high-entropy alloys identified by knowledge-based screening and valence electron concentration criteria",

(***)

H. Mizuseki*, R. Sahara, K. Hongo*,
**Comput. Mater. Sci.**, 267, 114584 (2026) [Q1-journal]
DOI : 10.1016/j.commatsci.2026.114584

* A207; "Superior Room-Temperature Gas Sensing Performance of Belt-like $VO_2$(B) over 1D $V_2O_5$ Nanofibers",

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Q. Cheng, L. Miao, P. Song, Q. Jin, A. Okawa, T. Hasegawa, K. Hongo, F. Tang, W. Cao, T.-W. Chiu, T. Sekino, S. Yin*,
**ACS Sens.**, 11, 1436-1446 (2026) [Q1-journal]
DOI : 10.1016/j.commatsci.2026.114512

* A206; "First–principles study of distance–dependent electronic coupling in TMD–metal interfaces",

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A. Ghaffar*, R. Maezono*, K. Hongo*,
**Comput. Mater. Sci.**, 265, 114512 (2025) [Q1-journal]
DOI : 10.1016/j.commatsci.2026.114512

* A205; "Facet-specific nitrogen vacancy engineering in BaMO2N (M = Ta, Nb) for enhanced electrochemical ammonia production: Insights from first-principles calculations",

(***)

C-C. Chu, Z-L. Li, K. Hongo, R. Maezono, Y. Masubuchi, J-C. Jianga*,
**Mater. Today Catal.**, 11, 100125 (2025) [Q1-journal]
DOI : 10.1016/j.mtcata.2025.100125

* A204; "Two-step W and N doping in $VO_2$: Synergistically reducing phase transition temperature while enhancing thermochromic performance",

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Y. Xue, L. Miao, P. Song, T. Hasegawa, A. Okawa, T. Sekino, R. Maezono, K. Hongo, S. Yin*,
**Chem. Eng. J.**, 522, 167980 (2025) [Q1-journal]
DOI : 10.1016/j.cej.2025.167980

* A203; "Ab *initio* screening for BCS-type superconductivity in $ThCr_2Si_2$-type compounds",
(***)

Tom Ichibha*, Ryo Maezono, Kenta Hongo,
**Phys. Scr.**, 100, 085969 (2025) [Q2-journal]
DOI : 10.1088/1402-4896/adf420

* A202; "Prediction of superconductivity in Haeckelite compounds using first-principles calculation",
(***)

K. Hamidi, M. Keivanloo, M. Sandoghchi, M. R. Mohammadizadeh, H. Raebiger, K. Hongo, R. Maezono, K. Ohno, M. Khazaei*,
**iScience**, 28, 113219 (2025) [Q1-journal]
DOI : 10.1016/j.isci.2025.113219

* A201; "Metal-Reduction-Triggered Red Luminescence Quenching in $Eu^{3+}$-Doped $Bi_2MoO_6$ Nanophosphors for $H_2S$ Gas Detection",
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T. Hangai, T. Hasegawa*, Y. Xue, A. Okawa, T. Ichibha, K. Hongo, R. Maezono, S. W. Kim, T. Goto, Y. Sato, S. Yin,
**ACS Appl. Nano Mater.**, 8, 12130-12139 (2025) [Q1-journal]
DOI : 10.1021/acsanm.5c01752

* A200; "Kinetic effects of ball-milling precursors on the synthesis pathway of KSbF4",
(酸素空孔を有する Ti ドープ ZnO 単層の NO ガスセンシングに関する第一原理解析)

R. Hisasue, T. Saquai, T. Ichiba, Y. Fujii, A. Yamashita, K. Hongo, R. Maezono, K. Tadanaga, A. Miura*,
**Ceram. Int.**, 51, 33653-33660 (2025) [Q1-journal]
DOI : 10.1016/j.ceramint.2025.05.096

* A199; "Density functional theory insights into NO gas sensing of Ti-doped ZnO monolayer with oxygen vacancy",
(酸素空孔を有する Ti ドープ ZnO 単層の NO ガスセンシングに関する第一原理解析)

Z. Mahmoudi, T. Ichibha, R. Maezono, M. Abbasnejad*,
**J. Appl. Phys.**, 137, 184303 (2025) [Q2-journal]
DOI : 10.1063/5.0256255

* A198; "Hand Milling Induced Phase Transition for Marcasite-type Carbodiimide",
(マルカサイト型カルボジイミドにおける手粉砕誘起の相転移)

Y. Yamamoto, K. Kume, S. Miyazaki, A. Shinozaki, P. Song, S. S. Hasan, K. Hongo, R. Maezono, H. Ubukata, H. Kageyama*, M. Higuchi, Y. Masubuchi*,
**J. Am. Chem. Soc.**, 147, 11390-11398 (2025) [Q1-journal]
DOI : 10.1021/jacs.5c00962

* A197; "Superconductivity in o-MAX phases",

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M. Keivanloo, M. Sandoghchi, M. R. Mohammadizadeh, M. Kawamura, H. Raebiger, K. Hongo, R. Maezono, M.Khazaei*,
**Nanoscale**, 17, 5341-5349 (2025) [Q1-journal]
DOI : 10.1039/D4NR04231J

* A196; "Quantum machine learning for $ABO_3$ perovskite structure prediction",

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M. Akrom*, S. Rustad*, H. K. Dipojono*, R. Maezono, H. Kasai,
**Comput. Mater. Sci.**, 250, 113694 (2025) [Q1-journal]
DOI : 10.1016/j.commatsci.2025.113694

* A195; "Nickel Vanadate Cathode Induced In Situ Phase Transition for Improved Zinc Storage by Low Migration Barrier and $Zn^{2+}/H^{+}$ Co-Insertion Mechanism",

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H. Bandi, A. K. Kakarla, R. Dahule, R. Maezono, D. Narsimulu, R. Shanthappa, J. S. Yu*,
**Small**, 21, (2025) [Q1-journal]
DOI : 10.1002/smll.202408568

* A194; "W/Mo/Cr Doping Modulates the Negative–Positive Inversion Gas Sensing Behavior of $VO_2$(M1)",

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L. Miao, Y. Xue, P. Song, T. Hasegawa, A. Okawa, R. Maezono, T. Sekino, S. Yin*,
**ACS Sens.**, 10, 526-536, (2025) [Q1-journal]
DOI : 10.1021/acssensors.4c03006

* A193; "Physics-informed Data-driven Discovery of Polymer Crystals with High Thermal Conductivity",

(***)

R. Dahule*, K. Oqmhula, R. Maezono, K. Hongo*,
**ACS Appl. Polym. Mater.**, 7, 1431-1439, (2025) [Q1-journal]
DOI : 10.1021/acsapm.4c03165

* A192; "Stability and Electronic Properties of SnS/ZnS Interfaces: A First-Principles Investigation",

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R. Dahule*, B. Gao, K. Hongo, Emila Panda, Yanming Ma, R. Maezono*,
**J. Phys. Chem. C.**, 129, 3158-3167, (2025) [Q1-journal]
DOI : 10.1021/acs.jpcc.4c06319

* A191; "Novel Selectivity: Target of Gas Sensing Defined by Behavior",

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L. Miao, P. Song, Y. Xue, Z. Hou, T. Hasegawa, A. Okawa, T. Goto, Y. Seo, R. Maezono, T. Sekino, S. Yin*,
**Adv. Mater.**, 37, 2413023, (2024) [Q1-journal]
DOI : 10.1002/adma.202413023

* A190; "A machine learning approach for forecasting the efficacy of pyridazine corrosion inhibitors",
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G. A. Trisnapradika, M. Akrom, S. Rustad, H. K. Dipojono, R. Maezono, H. Kasai*,
**Theor. Chem. Acc.**, 144, 8, (2024) [Q3-journal]
DOI : 10.1007/s00214-024-03165-2

* A189; "Theoretical Insights into High-$T_c$ Superconductivity of Structurally Ordered $YThH_{18}$: A First-Principles Study",
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A. Ghaffar*, P. Song, R. Maezono, K. Hongo*,
**ACS Omega**, 9, 49470-49479, (2024) [Q2-journal]
DOI : 10.1021/acsomega.4c07199

* A188; "Computational Study of the Structural, Mechanical, Electronic, Optical and Thermal properties of BaLiX (X =P, As, Sb) perovskites",
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M. Z. Rahman, S. S. Hasan, M. S. Akter, N. M. Mukhtar, N. Absar, M. A. Hasan, T. Ichibha, R. Maezono, K. Hongo, M. A. Islam*,
**Phys. B (Amsterdam, Neth.)**, 692, 416387 , (2024) [Q2-journal]
DOI : 10.1016/j.physb.2024.416387

* A187; "Using reinforcement learning to autonomously identify the source of errors for agents in group missions",
(原因系を効率よく切り分ける検証行動計画を自動的に策定する強化学習)

K. Utimula*, K-T. Hayaschi, T. J. Bihl, K. Nakano, K. Hongo, R. Maezono,
**Front. Control Eng.**, 5, (2024) [Q2-journal]
DOI : 10.3389/fcteg.2024.1402621

* A186; "Solid-liquid phase boundary of oxide solid solutions using neural network potentials",
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K. Hyodo, K. Hongo, T. Ichibha, R. Maezono*,
**J. Alloys Compd.**, 1006, 176227, (2024) [Q1-journal]
DOI : 10.1016/j.jallcom.2024.176227

* A185; "Unveiling the NIR modulation performance enhancement of $VO_2$ endowed by oxygen vacancy elimination",
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Y. Xue, L. Miao, P. Song, T. Hasegawa, A. Okawa, R. Maezono, T. Sekino, S. Yin*,
**Sol. Energy Mater. Sol. Cells.**, 274, 113007, (2024) [Q1-journal]
DOI : 10.1016/j.solmat.2024.113007

* A184; "Structural predictions and phonon-mediated superconductivity in platinum hydride under low pressure: Insight from first-principles calculations",
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P. Tsuppayakorn-aek, P. Song, W. Sukmas, R. Maezono, T. Bovornratanaraks,
**Comput. Mater. Sci.**, 244, 113265(2024) [Q1-journal]
DOI : 10.1016/j.commatsci.2024.113265

* A183; "Ca substitution effects on structure transformation and physical properties of (Eu,Ca)$FeAs_2$ co-doped with La and Co",
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S. P. K. Naik*, S. Alberto, K. Kataoka, Y. Gotoh, T. Ichibha, K. Hongo, R. Maezono, T. Nishio, H. Ogino*,
**Ceram. Int.**, 50, 40830-40838, (2024) [Q1-journal]
DOI : 10.1016/j.ceramint.2024.07.374

* A182; "Enhancing $MnBi_2Te_4$ Stability by Doping",
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K. Saritas*, A. Ghaffar, J. T. Krogel, T. Ichibha, K. Hongo, R. Maezono, F. A. Reboredo,
**J. Phys. Chem. C.**, 128, 10108-10119, (2024) [Q1-journal]
DOI : 10.1021/acs.jpcc.4c00848

* A181; "Thermal Decomposition of Oxygen-containing $Ta_3N_5$",
(タンタル窒化物への酸素ドープに関する状態図解析)

N. Moharana, C. Ghosh, A. Dasgupta, R. Maezono, S. Sarma, Ravi Kumar, K.C.Hari Kumar,
**J. Am. Ceram. Soc.**, 107, 6342-6352(2024) [Q1-journal]
DOI : 10.1111/jace.19869

* A180; "Substitutional Doping Strategies for Fermi Level Depinning and Enhanced Interface Quality in WS2-Metal Contacts",
(ドープした遷移金属ダイカルゴゲナイトの界面に関する第一原理解析)

A. Ghaffar, N.R. Mohapatra, K. Hongo, and R. Maezono,
**ACS Appl. Electron. Mater.**, 6, 4587-4600 (2024) [Q1-journal]
DOI : 10.1021/acsaelm.4c00609

* A179; "Key Role of Metal-to-Metal Charge Transfer Transition between $Mo^{6+}$ and $Bi^{3+}$ for Enhancement in NIR Luminescence of $Gd_2MoO_6$:Bi,Yb Nanophosphor",

(ナノ蛍光体の発光を増強させる金属イオン間の電荷移動)

T. Hangai, *T. Hasegawa, J. Xu, T. Nakanishi, T. Takeda, K. Nakano, K. Hongo, R. Maezono, T. Goto, Y. Sato, A. Okawa, S. Yin,
**J. Phys. Chem. C.** 128, 3351-3360 (2024) [Q1-journal]
DOI : 10.1021/acs.jpcc.3c07501

* A178; "Single crystal growth and physical properties of La, Co doped (Eu,Ca)$FeAs_2$",
(新規鉄系化合物単結晶の基礎物性解析)

*S. P. K. Naik, S. Alberto, K. Kataoka, Y. Gotoh, T. Ichibha, K. Hongo, R. Maezono, T. Nishio, *H. Ogino,
**J. Cryst. Growth.** 628, 127547 (2024) [Q2-journal]
DOI : 10.1016/j.jcrysgro.2023.127547

* A177; "Multi-emission of $Ce^{3+}$ from Single Crystallographic Site Induced by Disordering of Ions",
(秩序の乱れに起因した $Ce^{3+}$からの発光バリエーション)

T. Yasunaga, *M. Kobayashi, K. Oqmhula, H. Qi, T. Ichibha, K. Hongo, S. Yamamoto, R. Maezono, M. Mitsuishi, M. Osada, *H. Kato, M. Kakihana,
**Inorg. Chem.** 63, 1288－1295 (2024) [Q1-journal]
DOI : 10.1021/acs.inorgchem.3c03789

* A176; "Locality Error Free Effective Core Potentials for 3d Transition Metal Elements Developed for the Diffusion Monte Carlo Method",
(量子拡散モンテカルロ法用途の有効各電荷の開発--3d 遷移金属における局所近似誤差問題の解決)

*T. Ichibha, Y. Nikaido, C. M Bennett, J. T Krogel, K. Hongo, R. Maezono, *F. A Reboredo,
**J. Chem. Phys.** 159 164114 (2023) [Q1-journal]
DOI : 10.1063/5.0175381

* A175; "$(La,Th)H_{10}$: Potential high-$T_c$ (242 K) superconductors Stabilized Thermodynamically below 200 GPa",
(高圧下におけるランタン・トリウム水素化物の高温超伝導)

*P. Song, A. P. Durajski, Z. Hou, A. Ghaffar, R. Dahule, R. Szcze¸s´niak, K. Hongo, R. Maezono,
**J. Phys. Chem. C .** 128 2656–2665 (2024) [Q1-journal]
DOI : 10.1021/acs.jpcc.3c07213

* A174; "First-Principles Investigation of Stability and Superconductivity in Ternary Yttrium－Praseodymium Hydrides under High Pressure",
(遺伝的アルゴリズムを用いた高圧下の Y-Pr 水素化物における超伝導と合成安定性の予見)

*K. S. Qin, *P. Song, *K. Hongo, *R. Maezono,
**J. Phys. Chem. C** 127 21242-21249 (2023) [Q1-journal]
DOI : 10.1021/acs.jpcc.3c02968

* A173; "Structure, optical, and electrical properties of layered oxychalcogenide $Sr_2ZnCu_2(S_{1-x}Se_x)_2O_2$ ($0 \le x \le 1$) compounds",

(層状カルコゲナイト酸化物の構造と光学物性、電子物性)

T. Kato, Y. Iwasa, S. Pavan K. Naik, S. Ishida, Y. Higashi, I. Hase, T. Nishio, K. Hongo, R. Maezono, *H. Ogino,
**Mater. Res. Express** 10, 095904 (2023) [Q2-journal]
DOI : 10.1088/2053-1591/acf54d

* A172; "Recognition of spatial finiteness in meniscus splitting based on evaporative interface fluctuations",
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L. Wu, I. Saitoh, K. Hongo, *K. Okeyoshi,
**Adv. Mater. Interfaces** 2300510, 1-8 (2023) [Q1-journal]
DOI : 10.1002/admi.202300510

* A171; "Stiffer Bonding of Armchair Edge in Single-Layer Molybdenum Disulfide Nanoribbons",
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C. Liu, K. Hongo, R. Maezono, *J. Zhang, *Y. Oshima,
**ACS Appl. Mater. Interfaces** 10, 2303477 (2023) [Q1-journal]
DOI : 10.1002/advs.202303477

* A170; "Biophysical properties of fibril structure of the toxic conformer of amyloid-β42: characterization by atomic force microscopy and molecular docking",
(毒性型アミロイドベータのフィブリル構造に関するドッキングシミュレーションと原子力顕微鏡観測)

R. Biyani, K. Hirata, K. Oqhmhula, A. Yurtsever, K. Hongo, R. Maezono, M. Takagi, *T. Fukuma, *M. Biyani,
**ACS Appl. Mater. Interfaces,** 15, 27789–27800 (2023) [Q1-journal]
DOI : 10.1021/acsami.3c06460

* A169; "Existence of La-site antisite defects in $LaMO_3$ (M = Mn, Fe, and Co) predicted with many-body diffusion quantum Monte Carlo",
(LaMO3 型ペロブスカイト中アンチサイト欠陥 -- 量子拡散モンテカルロ法による存在予見)

T. Ichibha, S. Yoon, J. M. Ok, M. Yoon, H. N. Lee, F. A. Reboredo,
**Sci. Rep.,** 13 6703 (2023) [Q1-journal]
DOI : 10.1038/s41598-023-33578-1

* A168; "High-pressure BaCN2 phases explored by genetic algorithm",
(遺伝アルゴリズムを用いた金属カルボジイミド結晶の構造探索)

P. Song, M. Khawaguch, Y. Masubuchi, K. Oqmhula, K. Nakano, R. Maezono, K. Hongo,
**Comput. Mater. Sci.** 226 112202 (2023) [Q1-journal]
DOI : 10.1016/j.commatsci.2023.112202

* A167; "Evolutionary Algorithm Directed Synthesis of Mixed Anion Compounds LaF2X (X = Br, I) and LaFI2.",

(遺伝的アルゴリズムを援用したフッ化物複合アニオン物質の合成)

D. Kato, P. Song, H. Taguro, C. Tassel, H. Ubukata, K. Miyazaki, T. Abe, K. Nakano, T. Ichibha, K. Hongo, *R. Maezono, *H. Kageyama,,
**Angew. Chem. Int. Ed.** e202301416 (2023) [Q1-journal]
DOI : 10.1002/anie.202301416

* A166; "Towards chemical accuracy using the Jastrow correlated antisymmetrized geminal power ansatz",
(ジェミナル型多体波動関数で化学的精度を実現する電子状態計算)

A. Raghav, R. Maezono, K. Hongo, S. Sorella, K. Nakano,
**J. Chem. Theory Comput.** 19, 2222-2229 (2023) [Q1-journal]
DOI : 10.1021/acs.jctc.2c01141

* A165; "Thermodynamic Understanding of Impurity Phase Segregation in a PdCrO2/CuCrO2 Heterostructure",
(LaMO3 型ペロブスカイト中アンチサイト欠陥 -- 量子拡散モンテカルロ法による存在予見)

T. Ichibha, S. Yoon, J. M. Ok, M. Yoon, H. N. Lee, F. A. Reboredo,
**Advanced Physics Research** (2023) ,
DOI : 10.1002/apxr.202200080

* A164; "First-Principles-Based Insight into Electrochemical Reactivity in A Cobalt-Carbonate-Hydrate Pseudocapacitor",
(電気化学キャパシタ材料の蓄電特性をスーパーコンピュータを用いたシミュレーションで解明)

K. Oqmhula, T. Toma, R. Maezono, K. Hongo,
**ACS Omega** 8, 6743-6752 (2023) [Q1-journal]
DOI : 10.1021/acsomega.2c07362

* A163; "Mechanistic insights and importance of hydrophobicity in cationic polymers for cancer therapy",
(抗ガン高分子の分子設計指針に新たな光～カチオン性と疎水性の相乗効果で高い細胞障害性が発現～)

N. Kumar, K. Oqmhula, K. Hongo, K. Takagi, S. Yusa, R. Rajan, K. Matsumura,
**J. Mater. Chem. B.** 11, 1456-1468 (2023) [Q1-journal]
DOI : 10.1039/D2TB02059A

* A162; "Order–disorder competition in equiatomic 3d–transition–metal quaternary alloys: Phase stability and electronic structure",
(3d 遷移金属等組成 4 元系合金における秩序-無秩序競合：相安定性と電子状態)

H. Mizuseki, R. Sahara, K. Hongo,
**Sci. Technol. Adv. Mater.** 3, 2153632 (2023) [Q1-journal]
DOI : 10.1080/27660400.2022.2153632

* A161; "Electronic and magnetic properties of pure and Cu doped non-polar ZnO($10\bar{1}0$) surfaces",

(Cu をドープした ZnO 表面の電気的磁気的性質に関する第一原理解析)

E. Irandegani, R. Maezono, M. Abbasnejad,
**J. Appl. Phys.** 132 173903 (2022) [Q2-journal]
DOI : 10.1063/5.0106799

* A160; "Feature space of XRD patterns constructed by auto-encorder",
(オートエンコーダによって構成された XRD パターンの特徴量空間)

K. Utimula, M. Yano, H. Kimoto, K. Hongo, K. Nakano, R. Maezono,
**Adv. Theory Simul.** 2200613, (2022) [Q1-journal]
DOI : 10.1002/adts.202200613

* A159; " Potential high-$T_c$ superconductivity in $YCeH_{20}$ and $LaCeH_{20}$ under pressure",
(Ce 系水素化物の高圧化超伝導)

P. Song, Z. Hou, K. Nakano, K. Hongo, R. Maezono,
**Mater. Today Phys.**, 28 100873 (2022) [Q1-journal]
DOI : 10.1016/j.mtphys.2022.100873

* A158; "Anionic ordering in $Pb_2Ti_4O_9F_2$ revisited by nuclear magnetic resonance and density functional theory",
(鉛酸フッ化物のローンペアで安定化されるアニオン秩序配列)

K. Oka, T. Ichibha, D. Kato, M. Iwasaki, N. Noma, K. Hongo, R. Maezono, F. A. Reboredo,
**Dalton Trans. 51, 15361-15369**, (2022) [Q1-journal]
DOI : 10.1039/D2DT00839D

* A157; "Ab-initio-based Interface Modeling and Statistical Analysis for Estimate of the Water Contact Angle on a Metallic Cu(111) Surface",
(第一原理計算による界面モデリング:金属表面に対する接触角評価)

T. Murono, K. Hongo, K. Nakano, R. Maezono,
**Surf. Interfaces** 34, 102342 (2022) [Q1-journal]
DOI : 10.1016/j.surfin.2022.102342

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(ドープしたチタン酸化物の DFT+U 電子状態計算と有効質量解析)

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