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原著論文/著書リスト

原著論文/全て査読有(A174 以下が採録決定済/A181 以下が arXiv 済)

* A181; " Topological data analysis for revealing structural origin of density anomalies in silica glass", (***)

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

* A180; " 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)

* A179; " 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)

* A178; "Reinforcement learning autonomously identifying the source of errors for agents in a group mission",
(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. Hayaschi, K. Nakano, K. Hongo, R. Maezono,
arXiv:2107.09232 (2021)

* A177; "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)

* A176; "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

*A175; "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)

* A174; "Locality Error Free Effective Core Potentials for 3d Transition Metal Elements Developed for the Diffusion Monte Carlo Method",
(***)

*T. Ichibha, Y. Nikaido, C. M Bennett, J. T Krogel, K. Hongo, R. Maezono, *F. A Reboredo,
J. Chem. Phys. (2023) (2022/IF=4.4),
DOI : 10.1063/5.0175381

* A173; "(La,Th)H10: the Potential high-Tc (242 K) superconductors Stabilized Thermodynamically below 200 GPa",
(***)

*P. Song, A. P. Durajski, Z. Hou, A. Ghaffar, R. Dahule, R. Szcze̜śniak, K. Hongo, R. Maezono,
ACS Appl. Mater. Interfaces (2023) (2022/IF=9.5),
DOI : ***

* A172; "First-Principles Investigation of Stability and Superconductivity in Ternary Yttrium－Praseodymium Hydrides under High Pressure",
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*K. S. Qin, *P. Song, *K. Hongo, *R. Maezono,
J. Phys. Chem. C (2023) (2021/IF=4.177),
DOI : 10.1021/acs.jpcc.3c02968

* A171; "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 (2023) (2022/IF=5.4),
DOI : 10.1002/admi.202300510

* A170; "Biophysical properties of fibril structure of the toxic conformer of amyloid-β42: characterization by atomic force microscopy and molecular docking",
(***)

R. Biyani, K. Hirata, K. Oqhmhula, A. Yurtsever, K. Hongo, R. Maezono, M. Takagi, *T. Fukuma, *M. Biyani,
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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) (2021/IF=4.380),
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) (2022/IF=3.3),
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* A167; "Evolutionary Algorithm Directed Synthesis of Mixed Anion Compounds LaF2X (X = Br, I) and LaFI2.",
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D. Kato, P. Song, H. Taguro, C. Tassel, H. Ubukata, K. Miyazaki, T. Abe, K. Nakano, T. Ichibha, K. Hongo, *R. Maezono, *H. Kageyama,,
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* 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,
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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)

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* 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,

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* 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,
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* 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,
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* 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) (2022/IF=3.2)
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* 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)

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* 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)

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* 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,
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* 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,
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* A156; " Electronic structure and effective mass analysis of doped TiO_2 (anatase) systems using DFT+U",
(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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* A155; "Ab initio molecular dynamics simulation of structural and elastic properties of SiO2-P2O5-Al2O3 glass",
(ガラス材料の力学特性に関する第一原理分子動力学解析)

Y. Qian, B. Song, J. Jin, G. I. Prayogo, K. Utimula, K. Nakano, R. Maezono, K. Hongo, G. Zhao,
J. Am. Ceram. Soc. 105, 6604-6615(2022) (2022/IF=3.9)
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* A154; "High pressure hydrogen by machine learning and quantum Monte Carlo",
(厳密な電子状態計算 × 機械学習ポテンシャル:高圧水素における液体-液体相転移の研究)

A. Tirelli, G. Tenti, K. Nakano, S. Sorella,
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DOI : 10.1103/PhysRevB.106.L041105

* A153; " SHRY: Application of canonical augmentation to the atomic substitution problem",
(SHRY:正準強化法の原子置換問題への応用)

I. Prayogo, A. Tirelli, K. Utimula, K. Hongo, R. Maezono, K. Nakano,
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* A152; " High pressure behavior of tetragonal barium carbodiimide, BaNCN",
(カルボジイミド無機化合物の結晶構造の X 線回折および密度汎関数法による解析)

Y. Masubuchi, S. Miyazaki, P. Song, T. Yamamoto, K. Nakano, K. Hongo, R. Maezono,
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(元素置換による LiNiO2 の熱安定化)リチウムイオン電池の熱暴走を抑制するナノレベル材料設計)

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* A150; "Impact of Surface Faceting on Gas Sensing Selectivity of NiO: Revealing the Adsorption Sites of Organic Vapors on the {111} Facet",
(NiO(111)面のガス吸着選択性)

A. Hermawan, A. T. Hanindriyo, K. Hongo, R. Maezono, S. Yin,
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* A149; " Lattice Dynamics in the NASICON NaZr2(PO4)3 Solid Electrolyte from Temperature-Dependent Neutron Diffraction, NMR, and Ab Initio Computational Studies",
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(特異な熱電効率を示すバイオポリベンザゾールの物質設計)

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(拡散量子モンテカルロ法に基づく窒化ホウ素結晶多形の相対的安定性の研究)

Y. Nikaido, T. Ichibha, K. Hongo, F. A. Reboredo, K.C. H. Kumar , P. Mahadevan, R. Maezono, K. Nakano,
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(太陽電池材料・硫化スズの電子物性における格子欠陥の影響)

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(Mg-Sc-H 化合物系における高圧構造の安定性と高温超伝導発現機構の系統的研究)

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* A143; "Diffusion Monte Carlo evaluation of Disiloxane linearization barrier",
(スーパーコンピュータを活用して分子構造シミュレーション上の有名な難問を解決)

A. T. Hanindriyo, A. K. S. Yadav, T. Ichibha, R. Maezono, K. Nakano, K. Hongo,
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* A142; "Space-warp coordinate transformation for efficient ionic force calculations in quantum Monte Carlo",
(物質中の原子に働く力を高精度かつ高速に評価する手法を開発)

K. Nakano, A. Raghav, S. Sorella,
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(Y-Mg 系三元水素化物高温超伝導体の構造安定性に関する系統的研究)

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* A140; "Candidate Structure of the H2-PRE Phase of Solid Hydrogen",
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* A139; "High-T_c superconducting hydrides formed by the cage structures LaH_{24} and YH_{24} as basic blocks"
(ケージ構造 LaH_{24}, YH_{24} を基本ブロックとした超伝導水素化物)

P. Song, H. Zhufeng, P. Baptista de Castro, K. Nakano, K. Hongo, Y. Takano, R. Maezono,
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* A138; "Site-selective Eu^{3+} Luminescence in Monoclinic Phase of $YSiO_2N$"
(イットリウム蛍光体における発光増強)

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* A137; "Importance of van der Waals interactions in hydrogen adsorption on a silicon-carbide nanotube revisited with vdW-DFT and quantum Monte Carlo"
(SiC ナノチューブへの水素分子の吸着)

G. I. Prayogo, H. Shin, A. Benali, R. Maezono, K. Hongo,
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* A136; "Peculiar Atomic Bond Nature in Platinum Monatomic Chains"
(1 次元単原子鎖の力学的強度に関する解析)

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(LiNi1－xXxO2 における放電プロファイルの網羅的な 第一原理計算)

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* A134; "CrI3 revisited with a many-body ab initio theoretical approach"
(第一原理多体手法によるヨウ化クロムの層間相互作用評価)

T. Ichibha, A. L. Dzubak, J. T. Krogel, V. R. Cooper, and F. A. Reboredo,
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* A133; "Exploring diamondlike lattice thermal conductivity crystals via feature-based transfer learning"
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(量子アニーリングを用いた固体中イオン拡散の取扱い)

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(黒鱗半導体の電極に関する第一原理計算)

A. Ghaffar, M. D. Ganeriwala, K. Hongo, R. Maezono, N. R. Mohapatra,
ACS Omega. 6, 7795–7803 (2021) (2022/IF=4.1)
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(炭素ドーピングで誘起される酸素欠陥媒介チタン酸化物ナノ結晶の合成)

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J. Catal. 393, 179-189(2021) (2022/IF=7.3)
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* A128; "Atomic forces by quantum Monte Carlo: application to phonon dispersion calculation"
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* A127; "Exploring Heat-Shielding Nanoparticle-Based Materials Via First-Principles Calculations and Transfer Learning",
(転移学習を用いた熱遮材料の探索)

T. Yoshida, R. Maezono, and K. Hongo,
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engine,
(膨大なサンプルをクラスタリングするための, 確率的なクラスタ数推定方法)

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(BaTi2Pn2O (Pn = As, Sb)における圧力によって誘起される特異な Pn-Pn の伸長を伴う構造相転移)

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