

# 原著論文/著書リスト

原著論文/全て査読有 (A135 以下が採録決定済/A147 以下が arXiv 済)

- \* A147; "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)

- \* A146; "High-pressure Mg-Sc-H phase diagram and its superconductivity from first-principles calculations",  
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[P. Song](#), [Z. Hou](#), [P. B. d. Castro](#), [K. Nakano](#), [K. Hongo](#), [Y. Takano](#), [R. Maezono](#),  
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- \* A145; "The systematic study on the stability and superconductivity of Y-Mg-H compounds under high pressure",  
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[P. Song](#), [Z. Hou](#), [P. B. d. Castro](#), [K. Nakano](#), [K. Hongo](#), [Y. Takano](#), [R. Maezono](#),  
arXiv: 2107.05498 (2021)

- \* A144; "Novel superconducting clathrate structures in LaYH<sub>12</sub>",  
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[P. Song](#), [Z. Hou](#), [P. B. d. Castro](#), [K. Nakano](#), [K. Hongo](#), [Y. Takano](#), [R. Maezono](#),  
arXiv:2103.06690 (2021)

- \* A143; "High- $T_c$  ternary metal hydrides, YKH<sub>12</sub> and LaKH<sub>12</sub>, discovered by machine learning",  
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[P. Song](#), [H. Zhufeng](#), [P. Baptista de Castro](#), [K. Nakano](#), [K. Hongo](#), [Y. Takano](#), [R. Maezono](#),  
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- \* A142; "Diffusion Monte Carlo evaluation of Disiloxane linearization barrier",  
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[A. T. Hanindriyo](#), [A. K. S. Yadav](#), [T. Ichibha](#), [R. Maezono](#), [K. Nakano](#), [K. Hongo](#),  
arXiv:2009.11497 (2021)
- \* A141; "Interface modelling for ab initio evaluation of contact angle on a metallic 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. Muro](#), [K. Hongo](#), [K. Nakano](#), [R. Maezono](#),  
arXiv:2009.11497 (2020)
- \* A140; "Feature space of XRD patterns constructed by auto-encoder",  
(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](#),  
arXiv:2005.11660 (2020)
- \* A139; "First Principles Calculations of Superconducting Critical Temperature of ThCr<sub>2</sub>Si<sub>2</sub>-Publisher Structure",  
(ThCr<sub>2</sub>Si<sub>2</sub> 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 (2018/IF= 4.309))  
[arxiv.org/abs/1911.10716](https://arxiv.org/abs/1911.10716)
- \* A138; " Making the most of data: Quantum Monte Carlo Post-Analysis Revisited",  
(マルコフ鎖量子モンテカルロ法の効率的なリブロッキング処理)  
[T. Ichibha](#), [K. Hongo](#), [R. Maezono](#), [A.J.W. Thom](#),  
(submitted to Phys.Rev.E/IF = 2.284)  
[arxiv.org/abs/1904.09934](https://arxiv.org/abs/1904.09934) (2019)
- \* A137; "Importance of vdW and long-range exchange interactions to DFT-predicted docking energies between plumbagin and cyclodextrins"  
(シクロテ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)
- \* A136; "High T<sub>c</sub> superconducting hydrides formed by the cage structures LaH<sub>24</sub> and YH<sub>24</sub> as basic blocks",  
(ケージ構造 LaH<sub>24</sub>, YH<sub>24</sub> 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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\* A135; "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)

Genki Imam Prayogo, Hyeondeok Shin, Anouar Benali, [Ryo Maezono](#), [Kenta Hongo](#),  
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\* A133; "High-throughput evaluation of discharge profile of LiNi<sub>1-x</sub>Co<sub>x</sub>O<sub>2</sub> by ab initio calculations"

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\* A132; "Surface Study of Cu<sub>2</sub>SnS<sub>3</sub> Using First - Principles Density Functional Theory"

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R. Dahule, [A. Raghav](#), [A. T. Hanindriyo](#), [K. Hongo](#), [R. Maezono](#), E. Paanda,  
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\* A131; "A Quantum Annealing Approach to Ionic Diffusion in Solids"

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Z. Gu, Z. Cui, Z. Wang, K. S. Qin, Y. Asakura, T. Hasegawa, [K. Hongo](#), [R. Maezono](#), S. Yin,  
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\* A128; "Atomic forces by quantum Monte Carlo: application to phonon dispersion calculation"

(量子モンテカルロ法による力の計算: フォノン分散計算への応用)

[K. Nakano](#), T. Morresi, M. Casula, [R. Maezono](#), S. Sorella,  
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\* A126; "Stochastic estimations of a total number of classes for the clusterings with too enormous samples to be accommodate into a clustering engine,

(膨大なサンプルをクラスタリングするための、確率的なクラス数推定方法)

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- \* A124; "GaN bandgap bias caused by semi-core treatment in pseudopotentials analyzed by the diffusion Monte Carlo method",  
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[Y. Nikaido](#), [T. Ichibha](#), [K. Nakano](#), [K. Hongo](#), [R. Maezono](#),  
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- \* A123; "Synthesis, Electronic Structure, and Physical Properties of Layered Oxypnictides Sr<sub>2</sub>ScCrAsO<sub>3</sub> and Ba<sub>3</sub>Sc<sub>2</sub>Cr<sub>2</sub>As<sub>2</sub>O<sub>5</sub>",  
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(密度汎関数法によるアナターゼの欠陥準位解析)  
[A. Raghay](#), [A.T. Hanindriyo](#), [K. Utimula](#), [M. Abbasnejad](#), [R. Maezono](#), and E. Panda,  
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- \* A120; "General correlated geminal ansatz for electronic structure calculations: exploiting Pfaffians in place of determinant",  
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[K. Oqmhula](#), [K. Hongo](#), [R. Maezono](#), [T. Ichibha](#),  
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- \* A116; "New layered perovskite family built from [CeTa<sub>2</sub>O<sub>7</sub>]<sup>-</sup> layers: coloring mechanism from unique multi-transitions",  
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(可視光による光触媒を目指した酸ハロゲン化アパタイトの合成と触媒能評価)  
[M. Nakamura](#), [K. Oqmhula](#), [K. Utimula](#), M. Eguchi, K. Oka, [K. Hongo](#), [R. Maezono](#), [K. Maeda](#)  
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- \* A113; "Synergy of Binary Substitution for Improving Cycle Performance in LiNiO<sub>2</sub> Revealed by ab Initio Materials Informatics",  
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[A.T. Hanindriyo](#), [S. Sridar](#), [K.C. Hari Kumar](#), [K. Hongo](#), [R. Maezono](#),  
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(水素発生反応にかかる可視光光触媒水素の合成)  
[T. Oshima](#), [T. Ichibha](#), [K. Oqmhula](#), [K. Hibino](#), [S. Yamashita](#), [K. Fuji](#), [Y. Miseki](#), [K. Hongo](#), [D. Lu](#),  
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[K. Nakano](#), [C. Attacalite](#), [M. Barborini](#), [L. Capriotti](#), [M. Casula](#), [E. Coccia](#), [M. Dagrada](#), [C. Genovese](#), [Y. Luo](#), [G. Mazzola](#), [A. Zen](#), [S. Sorella](#),  
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- \* A101; "Inconsistencies in ab initio evaluations of non-additive contributions of DNA stacking energies"  
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S. Ganesanpotti, T. Yajima, T. Tohyama, Z. Li, K. Nakano, Y. Nozaki, C. Tassel, Y. Kobayashi, and H. Kageyama  
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(BaTi<sub>2</sub>(Sb<sub>1-x</sub>Sn<sub>x</sub>)<sub>2</sub>O:異原子価置換による T<sub>c</sub> の上昇)  
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G. Hasegawa, T. Sato, K. Kanamori, K. Nakano, T. Yajima, Y. Kobayashi, H. Kageyama, T. Abe, and K. Nakanishi,  
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