Kousuke Nakano

List of Publications by Year
in descending order

49	973	516710 16	477307 29
papers	citations	h-index	g-index

50	50	50	1089
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Diffusion Monte Carlo evaluation of disiloxane linearisation barrier. Physical Chemistry Chemical Physics, 2022, , .	2.8	0
2	Space-warp coordinate transformation for efficient ionic force calculations in quantum Monte Carlo. Journal of Chemical Physics, 2022, 156, 034101.	3.0	5
3	High-Pressure Mgâ€“Scâ€“H Phase Diagram and Its Superconductivity from First-Principles Calculations. Journal of Physical Chemistry C, 2022, 126, 2747-2755.	3.1	17
4	The Systematic Study on the Stability and Superconductivity of Yâ€Mgâ€H Compounds under High Pressure. Advanced Theory and Simulations, 2022, 5, .	2.8	13
5	Diffusion Monte Carlo Study on Relative Stabilities of Boron Nitride Polymorphs. Journal of Physical Chemistry C, 2022, 126, 6000-6007.	3.1	6
6	Computational Design to Suppress Thermal Runaway of Li-Ion Batteries via Atomic Substitutions to Cathode Materials. ACS Applied Materials & Interfaces, 2022, , .	8.0	2
7	<scp>Shry</scp>: Application of Canonical Augmentation to the Atomic Substitution Problem. Journal of Chemical Information and Modeling, 2022, 62, 2909-2915.	5.4	6
8	Ab initio molecular dynamics simulation of structural and elastic properties of SiO₂–P₂O₅–Al₂O₃–Na₂O glass. Journal of the American Ceramic Society, 2022, 105, 6604-6615.	3.8	7
9	High-pressure hydrogen by machine learning and quantum Monte Carlo. Physical Review B, 2022, 106, .	3.2	13
10	GaN bandgap bias caused by semi-core treatment in pseudopotentials analyzed by the diffusion Monte Carlo method. AIP Advances, 2021, 11, 025225.	1.3	2
11	Stochastic Estimations of the Total Number of Classes for a Clustering having Extremely Large Samples to be Included in the Clustering Engine. Advanced Theory and Simulations, 2021, 4, 2000301.	2.8	4
12	A quantum annealing approach to ionic diffusion in solids. Scientific Reports, 2021, 11, 7261.	3.3	2
13	Atomic forces by quantum Monte Carlo: Application to phonon dispersion calculations. Physical Review B, 2021, 103, .	3.2	12
14	High-Throughput Evaluation of Discharge Profiles of Nickel Substitution in LiNiO2 by Ab Initio Calculations. Journal of Physical Chemistry C, 2021, 125, 14517-14524.	3.1	5
15	Pressure-Induced Collapse Transition in BaTi₂Pn₂O (Pn = As, Sb) with an Unusual Pnâ€“Pn Bond Elongation. Inorganic Chemistry, 2021, 60, 2228-2233.	4.0	4
16	High-T_c Superconducting Hydrides Formed by LaH₂₄ and YH₂₄ Cage Structures as Basic Blocks. Chemistry of Materials, 2021, 33, 9501-9507.	6.7	16
17	General Correlated Geminal Ansatz for Electronic Structure Calculations: Exploiting Pfaffians in Place of Determinants. Journal of Chemical Theory and Computation, 2020, 16, 6114-6131.	5.3	11
18	Hydride-Reduced Eu2SrFe2O6: A T-to-Tâ€² Conversion Enabling Fe2+ in Square-Planar Coordination. Inorganic Chemistry, 2020, 59, 12913-12919.	4.0	2

#	Article	IF	Citations
19	<scp>TurboRVB</scp>: A many-body toolkit for ab initio electronic simulations by quantum Monte Carlo. Journal of Chemical Physics, 2020, 152, 204121.	3.0	37
20	Speeding up ab initio diffusion Monte Carlo simulations by a smart lattice regularization. Physical Review B, 2020, 101, .	3.2	10
21	All-Electron Quantum Monte Carlo with Jastrow Single Determinant Ansatz: Application to the Sodium Dimer. Journal of Chemical Theory and Computation, 2019, 15, 4044-4055.	5.3	13
22	Highâ€Pressure Synthesis of A 2 NiO 2 Ag 2 Se 2 (A=Sr, Ba) with a Highâ€Spin Ni 2+ in Squareâ€Planar Coordination. Angewandte Chemie, 2019, 131, 766-769.	2.0	15
23	Highâ€Pressure Synthesis of A₂NiO₂Ag₂Se₂ (A=Sr, Ba) with a Highâ€Spin Ni²⁺ in Squareâ€Planar Coordination. Angewandte Chemie - International Edition, 2019, 58, 756-759.	13.8	25
24	Estimation of maximum absorption wavelength of polymethine dyes in visible and near-infrared region based on time-dependent density functional theory. Chemical Physics, 2019, 518, 15-24.	1.9	15
25	Assessing the performance of the Tranâ€“Blaha modified Beckeâ€“Johnson exchange potential for optical constants of semiconductors in the ultravioletâ€“visible light region. Journal of Applied Physics, 2018, 123, .	2.5	21
26	Hypervalent Bismuthides La₃MBi₅ (M = Ti, Zr, Hf) and Related Antimonides: Absence of Superconductivity. Inorganic Chemistry, 2017, 56, 5041-5045.	4.0	15
27	Valence Band Engineering of Layered Bismuth Oxyhalides toward Stable Visible-Light Water Splitting: Madelung Site Potential Analysis. Journal of the American Chemical Society, 2017, 139, 18725-18731.	13.7	144
28	Investigation into Structural Phase Transitions in Layered Titanium-Oxypnictides by a Computational Phonon Analysis. Inorganic Chemistry, 2017, 56, 13732-13740.	4.0	5
29	Phonon dispersions and Fermi surfaces nesting explaining the variety of charge ordering in titanium-oxypnictides superconductors. Scientific Reports, 2016, 6, 29661.	3.3	19
30	Electrical Properties of Epitaxial Thin Films of Oxyhydrides ATiO_{3â€“x}H_x (A = Ba and Sr). Chemistry of Materials, 2015, 27, 6354-6359.	6.7	40
31	Superconductivity in LaPd2As2 with a collapsed 122 structure. Journal of Alloys and Compounds, 2014, 613, 370-374.	5.5	12
32	Superconducting properties of BaTi2Pn2O (Pn= Sb, Bi). Physica C: Superconductivity and Its Applications, 2014, 504, 36-38.	1.2	3
33	LaPd2Sb2: A pnictide superconductor with CaBe2Ge2 type structure. Journal of Alloys and Compounds, 2014, 583, 151-154.	5.5	23
34	Hierarchically Porous Monoliths Based on N-Doped Reduced Titanium Oxides and Their Electric and Electrochemical Properties. Chemistry of Materials, 2013, 25, 3504-3512.	6.7	52
35	Synthesis and Physical Properties of the New Oxybismuthides BaTi₂Bi₂O and (SrF)₂Ti₂Bi₂O with ad¹Square Net. Journal of the Physical Society of Japan, 2013, 82, 013703.	1.6	43
36	TcEnhancement by Aliovalent Anionic Substitution in Superconducting BaTi2(Sb1-xSnx)2O. Journal of the Physical Society of Japan, 2013, 82, 074707.	1.6	18

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37	Two Superconducting Phases in the Isovalent Solid Solutions BaTi₂Pn₂O (Pn= As, Sb, and Bi). Journal of the Physical Society of Japan, 2013, 82, 093705 Muon spin relaxation and electron/neutron diffraction studies of BaTi<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow	1.6	39
38			