Tsuyoshi Miyazaki

List of Publications by Year
in descending order

70	2,305	236925 25	214800 47
papers	citations	h-index	g-index

72	72	72	1962
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Structural analysis based on unsupervised learning: Search for a characteristic low-dimensional space by local structures in atomistic simulations. Physical Review B, 2022, 105, .	3.2	4
2	First-Principles Study on the Stability and Electronic Structure of the Charge-Ordered Phase in Î±-(BEDT-TTF)2I3. Crystals, 2021, 11, 1109.	2.2	3
3	The investigation of methane storage at the Ni-MOF-74 material: a periodic DFT calculation. Physical Chemistry Chemical Physics, 2021, 23, 12270-12279.	2.8	5
4	Structural change of damaged polyethylene by beta-decay of substituted tritium using reactive force field. Japanese Journal of Applied Physics, 2021, 60, SAAB06.	1.5	4
5	Molecular dynamics study on DNA damage by tritium disintegration. Japanese Journal of Applied Physics, 2020, 59, SAAE01.	1.5	7
6	First-principles study of topologically protected vortices and ferroelectric domain walls in hexagonal YGaO3. Physical Review B, 2020, 102, .	3.2	10
7	First-principles study of the charge ordered phase in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î¹</mml:mi><mml:mo>â^'</mml:mo><mml:msub><mml:mi mathvariant="normal">D</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:msub><mml:mrow><mml:mo>(</mml:mo><mml:mte : Stability of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Ï€</mml:mi></mml:math> -electron deuterium coupled ordering i. Physical Review B, 2020, 101, .	3.2	6
8	Blue moon ensemble simulation of aquation free energy profiles applied to mono and bifunctional platinum anticancer drugs. Journal of Computational Chemistry, 2020, 41, 1973-1984.	3.3	7
9	Large scale and linear scaling DFT with the CONQUEST code. Journal of Chemical Physics, 2020, 152, 164112.	3.0	55
10	The pseudoatomic orbital basis: electronic accuracy and soft-mode distortions in ABO₃ perovskites. Electronic Structure, 2020, 2, 025002.	2.8	2
11	Highly accurate local basis sets for large-scale DFT calculations in conquest. Japanese Journal of Applied Physics, 2019, 58, 100503.	1.5	17
12	Gate controlling of quantum interference and direct observation of anti-resonances in single molecule charge transport. Nature Materials, 2019, 18, 357-363.	27.5	160
13	Machine Learning Forces Trained by Gaussian Process in Liquid States: Transferability to Temperature and Pressure. Journal of the Physical Society of Japan, 2019, 88, 044601.	1.6	9
14	High-accuracy large-scale DFT calculations using localized orbitals in complex electronic systems: the case of grapheneâ€“metal interfaces. Journal of Physics Condensed Matter, 2018, 30, 505901.	1.8	9
15	(Invited) Large-Scale DFT Study of Ge/Si 3D Nanoislands and Core-Shell Nanowires. ECS Transactions, 2018, 86, 269-279.	0.5	4
16	Structural properties of siliconâ€“germanium and germaniumâ€“silicon coreâ€“shell nanowires. Journal of Physics Condensed Matter, 2018, 30, 465303.	1.8	8
17	(Invited) Large-Scale DFT Study of Ge/Si 3D Nanoislands and Core-Shell Nanowires. ECS Meeting Abstracts, 2018, , .	0.0	0
18	Large-Scale First-Principles Simulation on Li-Intercalated Graphite. ECS Meeting Abstracts, 2018, , .	0.0	0

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19	Emergence of the Dirac Electron System in a Single-Component Molecular Conductor under High Pressure. Journal of the American Chemical Society, 2017, 139, 1770-1773.	13.7	52
20	Canonical-ensemble extended Lagrangian Bornâ€“Oppenheimer molecular dynamics for the linear scaling density functional theory. Journal of Physics Condensed Matter, 2017, 29, 405901.	1.8	14
21	Efficient Calculation of Electronic Structure Using O(N) Density Functional Theory. Journal of Chemical Theory and Computation, 2017, 13, 4146-4153.	5.3	21
22	Machine learning for atomic forces in a crystalline solid: Transferability to various temperatures. International Journal of Quantum Chemistry, 2017, 117, 33-39.	2.0	29
23	Development of Large-scale First-Principles Molecular Dynamics Method for the Study of Structural and Physical Properties of Materials in the Earth's Deep Interior. Review of High Pressure Science and Technology/Koatsuryoku No Kagaku To Gijutsu, 2017, 27, 189-197.	0.0	0
24	Linear-scaling first-principles molecular dynamics of complex biological systems with the Conquest code. Japanese Journal of Applied Physics, 2016, 55, 1102B1.	1.5	10
25	Fragment Model Study of Molecular Multiorbital System X[Pd(dmit)2]2. Journal of the Physical Society of Japan, 2015, 84, 044716.	1.6	11
26	First-principles study of hydrogen-bonded molecular conductor<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î²</mml:mi><mml:mo>â^'</mml:mo><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:msub><mml:mrow><mml:mo>(</mml:mo><mml:mtext> Physical Review B, 2015, 92, .	3.2	14
27	Formation of self-assembled multi-layer stable palladium nanoparticles for ligand-free coupling reactions. RSC Advances, 2015, 5, 676-683.	3.6	18
28	Optimized multi-site local orbitals in the large-scale DFT program CONQUEST. Physical Chemistry Chemical Physics, 2015, 17, 31427-31433.	2.8	25
29	Large-scale DFT simulations with a linear-scaling DFT code CONQUEST on K-computer. Journal of Advanced Simulation in Science and Engineering, 2014, 1, 87-97.	0.2	22
30	Pressure-Induced Metallic Conductivity in the Single-Component Molecular Crystal [Ni(dmit)2]. European Journal of Inorganic Chemistry, 2014, 2014, 3837-3840.	2.0	29
31	Stable and Efficient Linear Scaling First-Principles Molecular Dynamics for 10000+ Atoms. Journal of Chemical Theory and Computation, 2014, 10, 5419-5425.	5.3	43
32	Angle-resolved photoemission study of the electronic structure of the quantum spin liquidEtMe3Sb[Pd(dmit)2]2. Physical Review B, 2014, 89, .	3.2	3
33	Efficient Calculations with Multisite Local Orbitals in a Large-Scale DFT Code CONQUEST. Journal of Chemical Theory and Computation, 2014, 10, 4813-4822.	5.3	29
34	A quantum chemistry study of Dsâ€“Pa unnatural DNA base pair. International Journal of Quantum Chemistry, 2013, 113, 504-509.	2.0	2
35	Density-functional theory study of gramicidin A ion channel geometry and electronic properties. Journal of the Royal Society Interface, 2013, 10, 20130547.	3.4	10
36	Cation Dependence of the Electronic States in Molecular Triangular Lattice System Î²^{â€²}-X[Pd(dmit)₂]₂: A First-Principles Study. Journal of the Physical Society of Japan, 2013, 82, 033709.	1.6	30

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37	Quasiparticles and Fermi liquid behaviour in an organic metal. Nature Communications, 2012, 3, 1089.	12.8	11
38	mathcal{O}(N) methods in electronic structure calculations. Reports on Progress in Physics, 2012, 75, 036503.	20.1	432
39	Linear Scaling Constrained Density Functional Theory in CONQUEST. Journal of Chemical Theory and Computation, 2011, 7, 884-889.	5.3	36
40	Calculations for millions of atoms with density functional theory: linear scaling shows its potential. Journal of Physics Condensed Matter, 2010, 22, 074207.	1.8	92
41	Evidence for a ball-shaped cyclen cyclophane: an experimental and first principles study. Physical Chemistry Chemical Physics, 2009, 11, 6038.	2.8	12
42	Non-self-consistent Density-Functional Theory Exchange-Correlation Forces for GGA Functionals. Journal of Chemical Theory and Computation, 2009, 5, 1499-1505.	5.3	12
43	First-Principles Study of the Tilted Dirac Cone in Î±-(BEDT-TTF)₂I₃at Hydrostatic Pressures. Journal of the Physical Society of Japan, 2009, 78, 105001.	1.6	3
44	<I>A Special Issue on</I> Advances in Quantum Simulators and Quantum Design. Journal of Computational and Theoretical Nanoscience, 2009, 6, 2447-2450.	0.4	0
45	Pseudo-atomic orbitals as basis sets for the O(N) DFT code CONQUEST. Journal of Physics Condensed Matter, 2008, 20, 294206.	1.8	31
46	Accuracy of order-Ndensity-functional theory calculations on DNA systems using CONQUEST. Journal of Physics Condensed Matter, 2008, 20, 294201.	1.8	25
47	The Energetics of Hut-Cluster Self-Assembly in Ge/Si(001) from Linear-Scaling DFT Calculations. Journal of the Physical Society of Japan, 2008, 77, 123706.	1.6	18
48	Density functional calculations of Ge(105): Local basis sets andO(N)methods. Physical Review B, 2007, 76, .	3.2	16
49	Order-N first-principles calculations with the conquest code. Computer Physics Communications, 2007, 177, 14-18.	7.5	64
50	Theoretical Study of the Phase Diagram of Î²'-(BEDT-TTF)2AuCl2at Hydrostatic Pressure. Journal of the Physical Society of Japan, 2006, 75, 104702.	1.6	3
51	Recent progress with large-scaleab initio calculations: the CONQUEST code. Physica Status Solidi (B): Basic Research, 2006, 243, 989-1000.	1.5	181
52	First-Principles Study of Electronic Structure in Î±-(BEDT-TTF)2I3at Ambient Pressure and with Uniaxial Strain. Journal of the Physical Society of Japan, 2006, 75, 034704.	1.6	128
53	First-principles study of the pressure effects onÎ²â€²â^'(BEDTâ^'TTF)2AuCl2. Physical Review B, 2006, 73, .	3.2	9
54	First-principle Study of Au_{<I>n</I>} Small Particles on MgO(001). Hyomen Kagaku, 2005, 26, 604-610.	0.0	2

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55	Atomic force algorithms in density functional theory electronic-structure techniques based on local orbitals. Journal of Chemical Physics, 2004, 121, 6186-6194.	3.0	39
56	Migration-Enhanced Epitaxy of Cubic BN: AnAb InitioStudy. Japanese Journal of Applied Physics, 2004, 43, 4092-4100.	1.5	4
57	Epitaxial Growth of Cubic BN on Diamond: AnAb InitioStudy. Japanese Journal of Applied Physics, 2004, 43, 7944-7946.	1.5	4
58	Magic layer thickness in Bi ultrathin films on Si(1 1 1) surface. Applied Surface Science, 2004, 237, 80-85.	6.1	21
59	Phase Diagram of Î²'-(BEDT-TTF)2ICl2under High Pressure Based on the First-Principles Electronic Structure. Journal of the Physical Society of Japan, 2004, 73, 25-28.	1.6	15
60	First-principles study of pressure effects on the molecular solids(CH3)4X[M(dmit)2]2(X=N,PandM=Ni,Pd). Physical Review B, 2003, 68, .	3.2	17
61	Atomic and electronic structures of the high-pressure superconductorÎ²â€²â^'(BEDTâ^'TTF)2ICl2:A first-principles study of the pressure effects. Physical Review B, 2003, 68, .	3.2	28
62	Recent progress in linear scalingab initioelectronic structure techniques. Journal of Physics Condensed Matter, 2002, 14, 2781-2798.	1.8	141
63	Parallel sparse matrix multiplication for linear scaling electronic structure calculations. Computer Physics Communications, 2001, 137, 255-273.	7.5	42
64	First-principles study on the insulating state ofÎ±â€²â^'NaV2O5. Physical Review B, 1999, 59, R12723-R12727.	3.2	7
65	First-principles study of the electronic structure of the organic solids(CH3)4N[M(dmit)2]2(M=Niand) Tj ETQq1 1 0.784314 rgBT /Ove lo R5269-R5272.	3.2	39
66	Inverse versus Normal NiAs Structures as High-Pressure Phases of FeO and MnO. Physical Review Letters, 1998, 81, 1027-1030.	7.8	65
67	(DIâ^'DCNQI)2Cuas a unique member of the DCNQI-Cu family: A theoretical study of high-pressure phases. Physical Review B, 1997, 56, R477-R480.	3.2	12
68	First-principles theoretical study of metallic states of DCNQI-(Cu,Ag,Li) systems. Physical Review B, 1996, 54, 10452-10464.	3.2	54
69	First-Principles Theoretical Study of Metallic States of DCNQI-(Cu,Ag) Systems: Simplicity and Variety in Complex Systems. Physical Review Letters, 1995, 74, 5104-5107.	7.8	62
70	Self-interaction correction for an impurity resonance state in metals. Physical Review B, 1993, 48, 16992-17000.	3.2	6