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	mathcal{O}(N) methods in electronic structure calculations. Reports on Progress in Physics, 2012, 75, 036503.	20.1	432
2	Recent progress with large-scaleab initio calculations: the CONQUEST code. Physica Status Solidi (B): Basic Research, 2006, 243, 989-1000.	1.5	181
3	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
4	Recent progress in linear scalingab initioelectronic structure techniques. Journal of Physics Condensed Matter, 2002, 14, 2781-2798.	1.8	141
5	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
6	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
7	Inverse versus Normal NiAs Structures as High-Pressure Phases of FeO and MnO. Physical Review Letters, 1998, 81, 1027-1030.	7.8	65
8	Order-N first-principles calculations with the conquest code. Computer Physics Communications, 2007, 177, 14-18.	7.5	64
9	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
10	Large scale and linear scaling DFT with the CONQUEST code. Journal of Chemical Physics, 2020, 152, 164112.	3.0	55
11	First-principles theoretical study of metallic states of DCNQI-(Cu,Ag,Li) systems. Physical Review B, 1996, 54, 10452-10464.	3.2	54
12	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
13	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
14	Parallel sparse matrix multiplication for linear scaling electronic structure calculations. Computer Physics Communications, 2001, 137, 255-273.	7.5	42
15	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 R5269-R5272.	3.2	39
16	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
17	Linear Scaling Constrained Density Functional Theory in CONQUEST. Journal of Chemical Theory and Computation, 2011, 7, 884-889.	5.3	36
18	Pseudo-atomic orbitals as basis sets for the O(N) DFT code CONQUEST. Journal of Physics Condensed Matter, 2008, 20, 294206.	1.8	31

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19	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
20	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
21	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
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	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
24	Accuracy of order-Ndensity-functional theory calculations on DNA systems using CONQUEST. Journal of Physics Condensed Matter, 2008, 20, 294201.	1.8	25
25	Optimized multi-site local orbitals in the large-scale DFT program CONQUEST. Physical Chemistry Chemical Physics, 2015, 17, 31427-31433.	2.8	25
26	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
27	Magic layer thickness in Bi ultrathin films on Si(1 1 1) surface. Applied Surface Science, 2004, 237, 80-85.	6.1	21
28	Efficient Calculation of Electronic Structure Using O(N) Density Functional Theory. Journal of Chemical Theory and Computation, 2017, 13, 4146-4153.	5.3	21
29	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
30	Formation of self-assembled multi-layer stable palladium nanoparticles for ligand-free coupling reactions. RSC Advances, 2015, 5, 676-683.	3.6	18
31	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
32	Highly accurate local basis sets for large-scale DFT calculations in conquest. Japanese Journal of Applied Physics, 2019, 58, 100503.	1.5	17
33	Density functional calculations of Ge(105): Local basis sets andO(N)methods. Physical Review B, 2007, 76, .	3.2	16
34	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
35	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:mte Physical Review B, 2015, 92, .	3.2	14
36	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

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37	(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
38	Evidence for a ball-shaped cyclen cyclophane: an experimental and first principles study. Physical Chemistry Chemical Physics, 2009, 11, 6038.	2.8	12
39	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
40	Quasiparticles and Fermi liquid behaviour in an organic metal. Nature Communications, 2012, 3, 1089.	12.8	11
41	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
42	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
43	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
44	First-principles study of topologically protected vortices and ferroelectric domain walls in hexagonal YGaO3. Physical Review B, 2020, 102, .	3.2	10
45	First-principles study of the pressure effects onÎ²â€²â˜(BEDTâ˜TTF)2AuCl2. Physical Review B, 2006, 73, .	3.2	9
46	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
47	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
48	Structural properties of siliconâ€“germanium and germaniumâ€“silicon coreâ€“shell nanowires. Journal of Physics Condensed Matter, 2018, 30, 465303.	1.8	8
49	First-principles study on the insulating state ofÎ±â€²â˜NaV2O5. Physical Review B, 1999, 59, R12723-R12727.	3.2	7
50	Molecular dynamics study on DNA damage by tritium disintegration. Japanese Journal of Applied Physics, 2020, 59, SAAE01.	1.5	7
51	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
52	Self-interaction correction for an impurity resonance state in metals. Physical Review B, 1993, 48, 16992-17000.	3.2	6
53	First-principles study of the charge ordered phase in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:miÎ²</mml:mi><mml:moâ˜</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:miÏ€</mml:mi></mml:math> -electron deuterium coupled ordering i. Physical Review B, 2020, 101, .	3.2	6
54	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

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55	Migration-Enhanced Epitaxy of Cubic BN: AnAb InitioStudy. Japanese Journal of Applied Physics, 2004, 43, 4092-4100.	1.5	4
56	Epitaxial Growth of Cubic BN on Diamond: AnAb InitioStudy. Japanese Journal of Applied Physics, 2004, 43, 7944-7946.	1.5	4
57	(Invited) Large-Scale DFT Study of Ge/Si 3D Nanoislands and Core-Shell Nanowires. ECS Transactions, 2018, 86, 269-279.	0.5	4
58	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
59	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
60	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
61	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
62	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
63	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
64	First-principle Study of Au_{<I>n</I>} Small Particles on MgO(001). Hyomen Kagaku, 2005, 26, 604-610.	0.0	2
65	A quantum chemistry study of Dsâ€“Pa unnatural DNA base pair. International Journal of Quantum Chemistry, 2013, 113, 504-509.	2.0	2
66	The pseudoatomic orbital basis: electronic accuracy and soft-mode distortions in ABO₃ perovskites. Electronic Structure, 2020, 2, 025002.	2.8	2
67	<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
68	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
69	(Invited) Large-Scale DFT Study of Ge/Si 3D Nanoislands and Core-Shell Nanowires. ECS Meeting Abstracts, 2018, , .	0.0	0
70	Large-Scale First-Principles Simulation on Li-Intercalated Graphite. ECS Meeting Abstracts, 2018, , .	0.0	0