Takao Kotani

List of Publications by Year
in descending order

64 papers	4,281 citations	201674 27 h-index	110387 64 g-index
66 all docs	66 docs citations	66 times ranked	3590 citing authors

#	Article	IF	Citations
1	Quasiparticle Self-ConsistentGWTheory. Physical Review Letters, 2006, 96, 226402.	7.8	781
2	All-Electron Self-ConsistentGWApproximation: Application to Si, MnO, and NiO. Physical Review Letters, 2004, 93, 126406.	7.8	475
3	Quasiparticle self-consistent<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>method: A basis for the independent-particle approximation. Physical Review B, 2007, 76, .	3.2	364
4	Electronic and crystal structure of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">Cu</mml:mi><mml:mrow><mml:mn>2</mml:mn><mml:mo>â^’</mml:mo><mml:mi>x</mml:mi></mml:mrow><mml:mi mathvariant="normal">S</mml:mi></mml:mrow></mml:math>: Full-potential electronic structure calculations. Physical Review B, 2007, 76, .	3.2	230
5	AbÂInitioPrediction of Conduction Band Spin Splitting in Zinc Blende Semiconductors. Physical Review Letters, 2006, 96, 086405.	7.8	193
6	All-electronGWcalculation based on the LAPW method:â€,Application to wurtzite ZnO. Physical Review B, 2002, 66, .	3.2	184
7	All-electron GW approximation with the mixed basis expansion based on the full-potential LMTO method. Solid State Communications, 2002, 121, 461-465.	1.9	168
8	Adequacy of approximations inGWtheory. Physical Review B, 2006, 74, .	3.2	149
9	Model Construction and a Possibility of Cupratelike Pairing in a New <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msup><mml:mi>d</mml:mi><mml:mn>9</mml:mn></mml:msup></mml:math> Nickelate Superconductor <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mo		

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19	Accurate energy bands calculated by the hybrid quasiparticle self-consistent GW method implemented in the ecalj package. Japanese Journal of Applied Physics, 2016, 55, 051201.	1.5	59
20	Ab initiorandom-phase-approximation calculation of the frequency-dependent effective interaction between 3d electrons: Ni, Fe, and MnO. Journal of Physics Condensed Matter, 2000, 12, 2413-2422.	1.8	57
21	Spin wave dispersion based on the quasiparticle self-consistentGWmethod: NiO, MnO and Î±-MnAs. Journal of Physics Condensed Matter, 2008, 20, 295214.	1.8	55
22	Finite-temperature quasiparticle self-consistentGWapproximation. Physical Review B, 2006, 74, .	3.2	51
23	Many-body electronic structure of metallic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î±</mml:mi></mml:math>-uranium. Physical Review B, 2008, 78, .	3.2	39
24	Quasiparticle Self-Consistent GW Method Based on the Augmented Plane-Wave and Muffin-Tin Orbital Method. Journal of the Physical Society of Japan, 2014, 83, 094711.	1.6	39
25	Impact ionization rates for Si, GaAs, InAs, ZnS, and GaN in the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>approximation. Physical Review B, 2010, 81, .	3.2	34
26	All-electron quasiparticle self-consistent <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi mathvariant="italic">GW</mml:mi></mml:math> band structures for <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>SrTiO</mml:mi><mml:mn>3</mml:mn></mml:msub></m including lattice polarization corrections in different phases. Physical Review Materials, 2018, 2, .	2.4	32
27	Exact exchange potential band-structure calculations for simple metals: Li, Na, K, Rb, and Ca. Physical Review B, 1995, 52, 17153-17157.	3.2	28
28	Electronic properties of alkali-metal loaded zeolites: Supercrystal Mott insulators. Physical Review B, 2004, 69, .	3.2	27
29	Growth and characterization of epitaxial Ba(Zn1/3Ta2/3)O3 (100) thin films. Acta Materialia, 2009, 57, 432-440.	7.9	26
30	Quasiparticle self-consistentGWmethod: a short summary. Journal of Physics Condensed Matter, 2007, 19, 365236.	1.8	24
31	Structureâ€“dielectric property relationship for vanadium- and scandium-doped barium strontium titanate. Acta Materialia, 2007, 55, 2647-2657.	7.9	22
32	Role of nonlocality in exchange correlation for magnetic two-dimensional van der Waals materials. Physical Review B, 2020, 101, .	3.2	22
33	Density Functional Theory through Legendre Transformation. Progress of Theoretical Physics, 1994, 92, 833-862.	2.0	22
34	Optimized-effective-potential method with exact exchange and exact RPA correlation-3d metals. Journal of Magnetism and Magnetic Materials, 1998, 177-181, 569-570.	2.3	21
35	Quasiparticle self-consistent GW study of cuprates: electronic structure, model parameters and the two-band theory for Tc. Scientific Reports, 2015, 5, 12050.	3.3	20
36	Formulation of the Augmented Plane-Wave and Muffin-Tin Orbital Method. Journal of the Physical Society of Japan, 2015, 84, 034702.	1.6	18

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37	Quasiparticle self-consistent GW calculation of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Sr</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>SrRuO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review B, 2016, 93, .	3.2	17
38	Strain-induced conduction-band spin splitting in GaAs from first-principles calculations. Physical Review B, 2008, 78, .	3.2	16
39	Linearized Augmented Plane-Wave and Muffin-Tin Orbital Method with the PBE Exchangeâ€“Correlation: Applied to Molecules from H2 through Kr2. Journal of the Physical Society of Japan, 2013, 82, 124714.	1.6	14
40	Quasiparticle self-consistent<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math> of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi mathvariant="normal">LaNiO</mml:mi><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi mathvariant="normal">LaNiO</mml:mi><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>	3.2	14
41	Nearest-neighbor sp3s* tight-binding parameters based on the hybrid quasi-particle self-consistent GW method verified by modeling of type-II superlattices. Journal of Applied Physics, 2017, 121, .	2.5	14
42	GW quasiparticle band structure of CaB6. Journal of Physics and Chemistry of Solids, 2002, 63, 1595-1597.	4.0	13
43	Ballistic conductance calculation of atomic-scale nanowires of Au and Co. Nanotechnology, 2007, 18, 095709.	2.6	13
44	Optimized effective potential method for exact exchange energy applied to solids. Physica B: Condensed Matter, 1997, 237-238, 332-335.	2.7	12
45	Electronic and optical properties of IIIâ€“nitrides under pressure. Physica Status Solidi (B): Basic Research, 2009, 246, 570-575.	1.5	12
46	Low-energy coherent Stoner-like excitations inCaFe2As2. Physical Review B, 2011, 83, .	3.2	12
47	Effect of electron localization in theoretical design of Ni-Mn-Ga based magnetic shape memory alloys. Materials and Design, 2021, 209, 109917.	7.0	12
48	Model-Mapped RPA for Determining the Effective Coulomb Interaction. Journal of the Physical Society of Japan, 2017, 86, 044714.	1.6	11
49	Nearest-neighbor sp³d⁵s* tight-binding parameters based on the hybrid quasi-particle self-consistent GW method verified by modeling of type-II superlattices. Optical Materials Express, 2018, 8, 1569.	3.0	11
50	Re-examination of half-metallic ferromagnetism for doped LaMnO₃in a quasiparticle self-consistentGWmethod. Journal of Physics Condensed Matter, 2009, 21, 266002.	1.8	10
51	Band structures for short-period (InAs)_n(GaSb)_nsuperlattices calculated by the quasiparticle self-consistent GW method. Japanese Journal of Applied Physics, 2017, 56, 021201.	1.5	9
52	Model-mapped random phase approximation to evaluate superconductivity in the fluctuation exchange approximation from first principles. Physical Review B, 2019, 99, .	3.2	9
53	Unified description of cuprate superconductors using a four-band<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>d</mml:mi><mml:mtext>â^’</mml:mtext><mml:mi>p</mml:mi></mml:mrow></mml:math>Physical Review Research, 2021, 3, .	3.6	8
54	Breakdown of a gold nanowire between electrodes. Nanotechnology, 2007, 18, 424002.	2.6	7

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55	Finite electric-field approach to evaluate the vertex correction for the screened Coulomb interaction in the quasiparticle self-consistent <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mm method. Physical Review B, 2020, 101, .	3.2	5
56	Effects of thermal vibrations on the valence-electron density and the forbidden x-ray reflections in C and Si. Physical Review B, 1991, 44, 6131-6136.	3.2	4
57	Band structure and pressure-induced metallic transition in iodine â€“ GW calculation. High Pressure Research, 2014, 34, 215-221.	1.2	4
58	Magnetic force theory combined with quasi-particle self-consistent GW method. Journal of Physics Condensed Matter, 2019, 31, 405503.	1.8	4
59	Electronic Structure and Spin-wave Dispersion of Cu₂MnAl, Ni₂MnSn, and Pd₂MnSn Based on Quasi-particle Self-consistent GW Calculations. Journal of the Physical Society of Japan, 2020, 89, 034704.	1.6	3
60	Calculations of quasiâ€particle spectra of semiconductors under pressure. Physica Status Solidi (B): Basic Research, 2011, 248, 1096-1101.	1.5	2
61	Structural and electronic properties of YH₃at high pressure â€“ band calculation by the GW approximation. High Pressure Research, 2012, 32, 464-470.	1.2	1
62	Nonlinear Extension of the Dynamical Linear Response of Spin: Extended Heisenberg Model. Journal of the Physical Society of Japan, 2021, 90, 094710.	1.6	1
63	An Analytic Procedure for Evaluating Grain-Size and Grain-Aspect-Ratio Distribution in Polycrystalline Sintered Bodies Based on Monte Carlo Simulation. Journal of the Ceramic Society of Japan, 1992, 100, 1235-1238.	1.3	0
64	Comparison of Daily Reproduction of COVID-19 among Countries by a New Reproduction Index RW8. Journal of the Physical Society of Japan, 2020, 89, 124803.	1.6	0