

Yosuke Kanai

List of Publications by Year in descending order

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70
papers

2,271
citations

201674

27
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223800

46
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75
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75
docs citations

75
times ranked

2997
citing authors

#	ARTICLE	IF	CITATIONS
1	Role of Semiconducting and Metallic Tubes in P3HT/Carbon-Nanotube Photovoltaic Heterojunctions: Density Functional Theory Calculations. <i>Nano Letters</i> , 2008, 8, 908-912.	9.1	145
2	Insights on Interfacial Charge Transfer Across P3HT/Fullerene Photovoltaic Heterojunction from Ab Initio Calculations. <i>Nano Letters</i> , 2007, 7, 1967-1972.	9.1	136
3	Accurate atomistic first-principles calculations of electronic stopping. <i>Physical Review B</i> , 2015, 91, .	3.2	121
4	Mechanism of Thermal Reversal of the (Fulvalene)tetracarbonyldiruthenium Photoisomerization: Toward Molecular Solar-Thermal Energy Storage. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 8926-8929.	13.8	105
5	Tunable Semiconductors: Control over Carrier States and Excitations in Layered Hybrid Organic-Inorganic Perovskites. <i>Physical Review Letters</i> , 2018, 121, 146401.	7.8	103
6	Surface Reaction of Alkynes and Alkenes with H-Si(111): A Density Functional Theory Study. <i>Journal of the American Chemical Society</i> , 2004, 126, 15890-15896.	13.7	86
7	Plane-wave pseudopotential implementation of explicit integrators for time-dependent Kohn-Sham equations in large-scale simulations. <i>Journal of Chemical Physics</i> , 2012, 137, 22A546.	3.0	80
8	Role of Surface Termination on Hot Electron Relaxation in Silicon Quantum Dots: A First-Principles Dynamics Simulation Study. <i>Nano Letters</i> , 2015, 15, 6429-6433.	9.1	73
9	Site-Selective Passivation of Defects in NiO Solar Photocathodes by Targeted Atomic Deposition. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 4754-4761.	8.0	71
10	Plane-wave pseudopotential implementation and performance of SCAN meta-GGA exchange-correlation functional for extended systems. <i>Journal of Chemical Physics</i> , 2017, 146, 22A105.	3.0	66
11	Examining real-time time-dependent density functional theory nonequilibrium simulations for the calculation of electronic stopping power. <i>Physical Review B</i> , 2017, 96, .	3.2	60
12	Communication: Modeling of concentration dependent water diffusivity in ionic solutions: Role of intermolecular charge transfer. <i>Journal of Chemical Physics</i> , 2015, 143, 241101.	3.0	53
13	Atomistic Oxidation Mechanism of a Carbon Nanotube in Nitric Acid. <i>Physical Review Letters</i> , 2010, 104, 066401.	7.8	52
14	X-ray Transient Absorption and Picosecond IR Spectroscopy of Fulvalene(tetracarbonyl)diruthenium on Photoexcitation. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 7692-7696.	13.8	47
15	Testing the TPSS meta-generalized-gradient-approximation exchange-correlation functional in calculations of transition states and reaction barriers. <i>Journal of Chemical Physics</i> , 2006, 125, 234104.	3.0	46
16	Role of Charge Transfer in Water Diffusivity in Aqueous Ionic Solutions. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 2711-2716.	4.6	46
17	Electronic stopping power in liquid water for protons and H^{\pm} particles from first principles. <i>Physical Review B</i> , 2016, 94, .	3.2	46
18	Passivation of Nickel Vacancy Defects in Nickel Oxide Solar Cells by Targeted Atomic Deposition of Boron. <i>Journal of Physical Chemistry C</i> , 2016, 120, 16568-16576.	3.1	44

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19	Role of Four-Fold Coordinated Titanium and Quantum Confinement in CO ₂ Reduction at Titania Surface. <i>Journal of the American Chemical Society</i> , 2012, 134, 20266-20269.	13.7	41
20	Quantum Dynamics Simulation of Electrons in Materials on High-Performance Computers. <i>Computing in Science and Engineering</i> , 2014, 16, 54-60.	1.2	41
21	Free Energy Profile of NaCl in Water: First-Principles Molecular Dynamics with SCAN and B97X-V Exchange-Correlation Functionals. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 884-893.	5.3	41
22	Charge separation in nanoscale photovoltaic materials: recent insights from first-principles electronic structure theory. <i>Journal of Materials Chemistry</i> , 2010, 20, 1053-1061.	6.7	38
23	All-electron <i>ab initio</i> Bethe-Salpeter equation approach to neutral excitations in molecules with numeric atom-centered orbitals. <i>Journal of Chemical Physics</i> , 2020, 152, 044105.	3.0	38
24	Electronic stopping for protons and α particles from first-principles electron dynamics: The case of silicon carbide. <i>Physical Review B</i> , 2016, 94, .	3.2	37
25	Exploring the Potential of Fulvalene Dimetals as Platforms for Molecular Solar Thermal Energy Storage: Computations, Syntheses, Structures, Kinetics, and Catalysis. <i>Chemistry - A European Journal</i> , 2014, 20, 15587-15604.	3.3	35
26	K -Shell Core-Electron Excitations in Electronic Stopping of Protons in Water from First Principles. <i>Physical Review Letters</i> , 2019, 123, 066401.	7.8	34
27	Role of Molecular Conjugation in the Surface Radical Reaction of Aldehydes with H ⁺ Si(111): First Principles Study. <i>Journal of Physical Chemistry B</i> , 2005, 109, 18889-18894.	2.6	31
28	Electronic Excitation Dynamics in DNA under Proton and α -Particle Irradiation. <i>Journal of the American Chemical Society</i> , 2019, 141, 5241-5251.	13.7	27
29	Competing Mechanisms in the Optically Activated Functionalization of the Hydrogen-Terminated Si(111) Surface. <i>Journal of the American Chemical Society</i> , 2006, 128, 3892-3893.	13.7	24
30	Simulating electronic excitation and dynamics with real-time propagation approach to TDDFT within plane-wave pseudopotential formulation. <i>Journal of Chemical Physics</i> , 2021, 155, 100901.	3.0	24
31	Surface Radical Chain Reaction Revisited: Comparative Investigation of Styrene and 2,4-Dimethyl-Styrene on Hydrogenated Si(001) Surface from Density Functional Theory Calculations. <i>Journal of Physical Chemistry C</i> , 2010, 114, 3981-3986.	3.1	22
32	Antiferromagnetic structures and electronic energy levels at reconstructed NiO(111) surfaces: A DFT study. <i>Physical Review B</i> , 2015, 91, .	3.2	22
33	Temperature dependence of nuclear quantum effects on liquid water via artificial neural network model based on SCAN meta-GGA functional. <i>Journal of Chemical Physics</i> , 2020, 153, 044114.	3.0	22
34	Role of exchange in density-functional theory for weakly interacting systems: Quantum Monte Carlo analysis of electron density and interaction energy. <i>Physical Review A</i> , 2009, 80, .	2.5	21
35	Atom Transfer Radical Polymerization Preparation and Photophysical Properties of Polypyridylruthenium Derivatized Polystyrenes. <i>Inorganic Chemistry</i> , 2013, 52, 8511-8520.	4.0	21
36	A Theoretical Study of Biotin Chemisorption on Si ⁺ SiC(001) Surfaces. <i>Journal of Physical Chemistry B</i> , 2005, 109, 13656-13662.	2.6	20

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37	Size Dependence and Role of Decoherence in Hot Electron Relaxation within Fluorinated Silicon Quantum Dots: A First-Principles Study. <i>Journal of Physical Chemistry C</i> , 2018, 122, 29526-29536.	3.1	20
38	Propagation of maximally localized Wannier functions in real-time TDDFT. <i>Journal of Chemical Physics</i> , 2019, 150, 194113.	3.0	20
39	All-Electron BSE@ <i>GW</i> Method for <i>K</i> -Edge Core Electron Excitation Energies. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 1569-1583.	5.3	20
40	Electronic Excitation Dynamics in Liquid Water under Proton Irradiation. <i>Scientific Reports</i> , 2017, 7, 40379.	3.3	18
41	Excited Electron Dynamics at Semiconductor-Molecule Type-II Heterojunction Interface: First-Principles Dynamics Simulation. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 1495-1500.	4.6	17
42	Toward accurate reaction energetics for molecular line growth at surface: Quantum Monte Carlo and density functional theory calculations. <i>Journal of Chemical Physics</i> , 2009, 131, 214708.	3.0	16
43	Single-Molecule-Resolved Structural Changes Induced by Temperature and Light in Surface-Bound Organometallic Molecules Designed for Energy Storage. <i>ACS Nano</i> , 2011, 5, 3701-3706.	14.6	16
44	Nuclear Quantum Effect and Its Temperature Dependence in Liquid Water from Random Phase Approximation via Artificial Neural Network. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 6354-6362.	4.6	16
45	Biomimetic Carbon Nanotube for Catalytic CO ₂ Hydrolysis: First-Principles Investigation on the Role of Oxidation State and Metal Substitution in Porphyrin. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 1369-1373.	4.6	15
46	Examining the Effect of Exchange-Correlation Approximations in First-Principles Dynamics Simulation of Interfacial Charge Transfer. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2634-2641.	5.3	15
47	All-electron real-time and imaginary-time time-dependent density functional theory within a numeric atom-centered basis function framework. <i>Journal of Chemical Physics</i> , 2021, 155, 154801.	3.0	14
48	First-Principles Modeling of Electronic Stopping in Complex Matter under Ion Irradiation. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 229-237.	4.6	13
49	Quantum Monte Carlo calculations of the energy-level alignment at hybrid interfaces: Role of many-body effects. <i>Physical Review B</i> , 2009, 79, .	3.2	12
50	Theoretical oxidation state analysis of Ru-(bpy) ₃ : Influence of water solvation and Hubbard correction in first-principles calculations. <i>Journal of Chemical Physics</i> , 2014, 141, 024305.	3.0	11
51	Dynamical transition orbitals: A particle-hole description in real-time TDDFT dynamics. <i>Journal of Chemical Physics</i> , 2021, 154, 054107.	3.0	11
52	Excitation energy-dependent photocurrent switching in a single-molecule photodiode. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 16198-16203.	7.1	10
53	Enabling Aqueous NiO Photocathodes by Passivating Surface Sites That Facilitate Proton-Coupled Charge Transfer. <i>ACS Applied Energy Materials</i> , 2020, 3, 10702-10713.	5.1	10
54	Dependence of Water Dynamics on Molecular Adsorbates near Hydrophobic Surfaces: First-Principles Molecular Dynamics Study. <i>Journal of Physical Chemistry C</i> , 2014, 118, 8508-8513.	3.1	9

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55	Importance of Excitonic Effect in Charge Separation at Quantum-Dot/Organic Interface: First-Principles Many-Body Calculations. <i>Nano Letters</i> , 2014, 14, 6884-6888.	9.1	8
56	Theory and Simulation of Nanostructured Materials for Photovoltaic Applications. <i>Computing in Science and Engineering</i> , 2010, 12, 18-27.	1.2	7
57	Diffusion quantum Monte Carlo study of martensitic phase transition energetics: The case of phosphorene. <i>Journal of Chemical Physics</i> , 2016, 145, 124705.	3.0	7
58	Dependence of hot electron transfer on surface coverage and adsorbate species at semiconductor–molecule interfaces. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 12986-12991.	2.8	6
59	Modeling time-coincident ultrafast electron transfer and solvation processes at molecule-semiconductor interfaces. <i>Journal of Chemical Physics</i> , 2014, 140, 234109.	3.0	5
60	Reptation Quantum Monte Carlo calculation of charge transfer: The Na–Cl dimer. <i>Chemical Physics Letters</i> , 2015, 618, 236-240.	2.6	4
61	Modeling Electron Injection at Semiconductor–Molecule Interfaces using First-Principles Dynamics Simulation: Effects of Nonadiabatic Coupling, Self-energy, and Surface Models. <i>Journal of Physical Chemistry C</i> , 2019, 123, 13295-13303.	3.1	4
62	First-Principles Demonstration of Nonadiabatic Thouless Pumping of Electrons in a Molecular System. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 4496-4503.	4.6	4
63	Nonlinear electronic excitation in water under proton irradiation: a first principles study. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 5598-5603.	2.8	3
64	Nuclear–electronic orbital approach to quantization of protons in periodic electronic structure calculations. <i>Journal of Chemical Physics</i> , 2022, 156, .	3.0	3
65	Cooperative Chiral Adsorption of Styrene Molecules on the Si(001)- $\sqrt{2} \times \sqrt{2}$ Surface: First-Principles Investigation of Reaction Mechanisms. <i>Journal of Physical Chemistry C</i> , 2011, 115, 14213-14218.	3.1	2
66	First Principles Dynamics Study of Excited Hole Relaxation in DNA. <i>ChemPhysChem</i> , 2022, 23, .	2.1	2
67	Scaling and spatial analysis of the dielectric response of cadmium selenide nanowires. <i>Physical Review B</i> , 2014, 90, .	3.2	1
68	Modeling Plasmon-Induced Hot-Carrier Transfer. <i>CheM</i> , 2018, 4, 937-939.	11.7	1
69	QMC Assessments of Weak-interaction Described by DFT within various XC approximations / Effects of Carbon Nanotube Oxidation on Molecular Interactions. <i>Materials Research Society Symposia Proceedings</i> , 2008, 1084, 50301.	0.1	0
70	Electronic and optical properties of polypyridylruthenium derivatized polystyrenes: multi-level computational analysis of metallo-polymeric chromophore assemblies. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 1776-1784.	2.8	0