Yosuke Kanai

List of Publications by Year
in descending order

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70 papers	2,271 citations	201575 27 h-index	223716 46 g-index
75 all docs	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. Nano Letters, 2008, 8, 908-912.	4.5	145
2	Insights on Interfacial Charge Transfer Across P3HT/Fullerene Photovoltaic Heterojunction from Ab Initio Calculations. Nano Letters, 2007, 7, 1967-1972.	4.5	136
3	Accurate atomistic first-principles calculations of electronic stopping. Physical Review B, 2015, 91, .	1.1	121
4	Mechanism of Thermal Reversal of the (Fulvalene)tetracarbonyldiruthenium Photoisomerization: Toward Molecular Solarâ€“Thermal Energy Storage. Angewandte Chemie - International Edition, 2010, 49, 8926-8929.	7.2	105
5	Tunable Semiconductors: Control over Carrier States and Excitations in Layered Hybrid Organic-Inorganic Perovskites. Physical Review Letters, 2018, 121, 146401.	2.9	103
6	Surface Reaction of Alkynes and Alkenes with H-Si(111):Â A Density Functional Theory Study. Journal of the American Chemical Society, 2004, 126, 15890-15896.	6.6	86
7	Plane-wave pseudopotential implementation of explicit integrators for time-dependent Kohn-Sham equations in large-scale simulations. Journal of Chemical Physics, 2012, 137, 22A546.	1.2	80
8	Role of Surface Termination on Hot Electron Relaxation in Silicon Quantum Dots: A First-Principles Dynamics Simulation Study. Nano Letters, 2015, 15, 6429-6433.	4.5	73
9	Site-Selective Passivation of Defects in NiO Solar Photocathodes by Targeted Atomic Deposition. ACS Applied Materials & Interfaces, 2016, 8, 4754-4761.	4.0	71
10	Plane-wave pseudopotential implementation and performance of SCAN meta-GGA exchange-correlation functional for extended systems. Journal of Chemical Physics, 2017, 146, 224105.	1.2	66
11	Examining real-time time-dependent density functional theory nonequilibrium simulations for the calculation of electronic stopping power. Physical Review B, 2017, 96, .	1.1	60
12	Communication: Modeling of concentration dependent water diffusivity in ionic solutions: Role of intermolecular charge transfer. Journal of Chemical Physics, 2015, 143, 241101.	1.2	53
13	Atomistic Oxidation Mechanism of a Carbon Nanotube in Nitric Acid. Physical Review Letters, 2010, 104, 066401.	2.9	52
14	Xâ€ray Transient Absorption and Picosecond IR Spectroscopy of Fulvalene(tetracarbonyl)diruthenium on Photoexcitation. Angewandte Chemie - International Edition, 2012, 51, 7692-7696.	7.2	47
15	Testing the TPSS meta-generalized-gradient-approximation exchange-correlation functional in calculations of transition states and reaction barriers. Journal of Chemical Physics, 2006, 125, 234104.	1.2	46
16	Role of Charge Transfer in Water Diffusivity in Aqueous Ionic Solutions. Journal of Physical Chemistry Letters, 2014, 5, 2711-2716.	2.1	46
17	Electronic stopping power in liquid water for protons and Î± particles from first principles. Physical Review B, 2016, 94, .	1.1	46
18	Passivation of Nickel Vacancy Defects in Nickel Oxide Solar Cells by Targeted Atomic Deposition of Boron. Journal of Physical Chemistry C, 2016, 120, 16568-16576.	1.5	44

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19	Role of Four-Fold Coordinated Titanium and Quantum Confinement in CO₂ Reduction at Titania Surface. Journal of the American Chemical Society, 2012, 134, 20266-20269.	6.6	41
20	Quantum Dynamics Simulation of Electrons in Materials on High-Performance Computers. Computing in Science and Engineering, 2014, 16, 54-60.	1.2	41
21	Free Energy Profile of NaCl in Water: First-Principles Molecular Dynamics with SCAN and ï‰B97X-V Exchangeâ€“Correlation Functionals. Journal of Chemical Theory and Computation, 2018, 14, 884-893.	2.3	41
22	Charge separation in nanoscale photovoltaic materials: recent insights from first-principles electronic structure theory. Journal of Materials Chemistry, 2010, 20, 1053-1061.	6.7	38
23	All-electron ab initio Bethe-Salpeter equation approach to neutral excitations in molecules with numeric atom-centered orbitals. Journal of Chemical Physics, 2020, 152, 044105.	1.2	38
24	Electronic stopping for protons and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î±</mml:mi></mml:math>particles from first-principles electron dynamics: The case of silicon carbide. Physical Review B, 2016, 94, .	1.1	37
25	Exploring the Potential of Fulvalene Dimetals as Platforms for Molecular Solar Thermal Energy Storage: Computations, Syntheses, Structures, Kinetics, and Catalysis. Chemistry - A European Journal, 2014, 20, 15587-15604.	1.7	35
26	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>K</mml:mi></mml:mrow></mml:math> -Shell Core-Electron Excitations in Electronic Stopping of Protons in Water from First Principles. Physical Review Letters, 2019, 123, 066401.	2.9	34
27	Role of Molecular Conjugation in the Surface Radical Reaction of Aldehydes with Hâ^'Si(111):â€‰ First Principles Study. Journal of Physical Chemistry B, 2005, 109, 18889-18894.	1.2	31
28	Electronic Excitation Dynamics in DNA under Proton and Î±-Particle Irradiation. Journal of the American Chemical Society, 2019, 141, 5241-5251.	6.6	27
29	Competing Mechanisms in the Optically Activated Functionalization of the Hydrogen-Terminated Si(111) Surface. Journal of the American Chemical Society, 2006, 128, 3892-3893.	6.6	24
30	Simulating electronic excitation and dynamics with real-time propagation approach to TDDFT within plane-wave pseudopotential formulation. Journal of Chemical Physics, 2021, 155, 100901.	1.2	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. Journal of Physical Chemistry C, 2010, 114, 3981-3986.	1.5	22
32	Antiferromagnetic structures and electronic energy levels at reconstructed NiO(111) surfaces: A<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>DFT</mml:mi><mml:mo>+</mml:mo><mml:mi>U</mml:mi></mml:mrow></mml:math> Physical Review B, 2015, 91, .	1.1	22
33	Temperature dependence of nuclear quantum effects on liquid water via artificial neural network model based on SCAN meta-GGA functional. Journal of Chemical Physics, 2020, 153, 044114.	1.2	22
34	Role of exchange in density-functional theory for weakly interacting systems: Quantum Monte Carlo analysis of electron density and interaction energy. Physical Review A, 2009, 80, .	1.0	21
35	Atom Transfer Radical Polymerization Preparation and Photophysical Properties of Polypyridylruthenium Derivatized Polystyrenes. Inorganic Chemistry, 2013, 52, 8511-8520.	1.9	21
36	A Theoretical Study of Biotin Chemisorption on Siâ^'SiC(001) Surfaces. Journal of Physical Chemistry B, 2005, 109, 13656-13662.	1.2	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. Journal of Physical Chemistry C, 2018, 122, 29526-29536.	1.5	20
38	Propagation of maximally localized Wannier functions in real-time TDDFT. Journal of Chemical Physics, 2019, 150, 194113.	1.2	20
39	All-Electron BSE@GW Method for K-Edge Core Electron Excitation Energies. Journal of Chemical Theory and Computation, 2022, 18, 1569-1583.	2.3	20
40	Electronic Excitation Dynamics in Liquid Water under Proton Irradiation. Scientific Reports, 2017, 7, 40379.	1.6	18
41	Excited Electron Dynamics at Semiconductorâ€“Molecule Type-II Heterojunction Interface: First-Principles Dynamics Simulation. Journal of Physical Chemistry Letters, 2016, 7, 1495-1500.	2.1	17
42	Toward accurate reaction energetics for molecular line growth at surface: Quantum Monte Carlo and density functional theory calculations. Journal of Chemical Physics, 2009, 131, 214708.	1.2	16
43	Single-Molecule-Resolved Structural Changes Induced by Temperature and Light in Surface-Bound Organometallic Molecules Designed for Energy Storage. ACS Nano, 2011, 5, 3701-3706.	7.3	16
44	Nuclear Quantum Effect and Its Temperature Dependence in Liquid Water from Random Phase Approximation via Artificial Neural Network. Journal of Physical Chemistry Letters, 2021, 12, 6354-6362.	2.1	16
45	Biomimetic Carbon Nanotube for Catalytic CO₂ Hydrolysis: First-Principles Investigation on the Role of Oxidation State and Metal Substitution in Porphyrin. Journal of Physical Chemistry Letters, 2012, 3, 1369-1373.	2.1	15
46	Examining the Effect of Exchange-Correlation Approximations in First-Principles Dynamics Simulation of Interfacial Charge Transfer. Journal of Chemical Theory and Computation, 2017, 13, 2634-2641.	2.3	15
47	All-electron real-time and imaginary-time time-dependent density functional theory within a numeric atom-centered basis function framework. Journal of Chemical Physics, 2021, 155, 154801.	1.2	14
48	First-Principles Modeling of Electronic Stopping in Complex Matter under Ion Irradiation. Journal of Physical Chemistry Letters, 2020, 11, 229-237.	2.1	13
49	Quantum Monte Carlo calculations of the energy-level alignment at hybrid interfaces: Role of many-body effects. Physical Review B, 2009, 79, .	1.1	12
50	Theoretical oxidation state analysis of Ru-(bpy)3: Influence of water solvation and Hubbard correction in first-principles calculations. Journal of Chemical Physics, 2014, 141, 024305.	1.2	11
51	Dynamical transition orbitals: A particleâ€“hole description in real-time TDDFT dynamics. Journal of Chemical Physics, 2021, 154, 054107.	1.2	11
52	Excitation energy-dependent photocurrent switching in a single-molecule photodiode. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 16198-16203.	3.3	10
53	Enabling Aqueous NiO Photocathodes by Passivating Surface Sites That Facilitate Proton-Coupled Charge Transfer. ACS Applied Energy Materials, 2020, 3, 10702-10713.	2.5	10
54	Dependence of Water Dynamics on Molecular Adsorbates near Hydrophobic Surfaces: First-Principles Molecular Dynamics Study. Journal of Physical Chemistry C, 2014, 118, 8508-8513.	1.5	9

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55	Importance of Excitonic Effect in Charge Separation at Quantum-Dot/Organic Interface: First-Principles Many-Body Calculations. Nano Letters, 2014, 14, 6884-6888.	4.5	8
56	Theory and Simulation of Nanostructured Materials for Photovoltaic Applications. Computing in Science and Engineering, 2010, 12, 18-27.	1.2	7
57	Diffusion quantum Monte Carlo study of martensitic phase transition energetics: The case of phosphorene. Journal of Chemical Physics, 2016, 145, 124705.	1.2	7
58	Dependence of hot electron transfer on surface coverage and adsorbate species at semiconductorâ€“molecule interfaces. Physical Chemistry Chemical Physics, 2018, 20, 12986-12991.	1.3	6
59	Modeling time-coincident ultrafast electron transfer and solvation processes at molecule-semiconductor interfaces. Journal of Chemical Physics, 2014, 140, 234109.	1.2	5
60	Reptation Quantum Monte Carlo calculation of charge transfer: The Naâ€“Cl dimer. Chemical Physics Letters, 2015, 618, 236-240.	1.2	4
61	Modeling Electron Injection at Semiconductorâ€“Molecule Interfaces using First-Principles Dynamics Simulation: Effects of Nonadiabatic Coupling, Self-energy, and Surface Models. Journal of Physical Chemistry C, 2019, 123, 13295-13303.	1.5	4
62	First-Principles Demonstration of Nonadiabatic Thouless Pumping of Electrons in a Molecular System. Journal of Physical Chemistry Letters, 2021, 12, 4496-4503.	2.1	4
63	Nonlinear electronic excitation in water under proton irradiation: a first principles study. Physical Chemistry Chemical Physics, 2022, 24, 5598-5603.	1.3	3
64	Nuclearâ€“electronic orbital approach to quantization of protons in periodic electronic structure calculations. Journal of Chemical Physics, 2022, 156, .	1.2	3
65	Cooperative Chiral Adsorption of Styrene Molecules on the Si(001)-c(2 Ã— 4) Surface: First-Principles Investigation of Reaction Mechanisms. Journal of Physical Chemistry C, 2011, 115, 14213-14218.	1.5	2
66	First Principles Dynamics Study of Excited Hole Relaxation in DNA. ChemPhysChem, 2022, 23, .	1.0	2
67	Scaling and spatial analysis of the dielectric response of cadmium selenide nanowires. Physical Review B, 2014, 90, .	1.1	1
68	Modeling Plasmon-Induced Hot-Carrier Transfer. CheM, 2018, 4, 937-939.	5.8	1
69	QMC Assessments of Weak-interaction Described by DFT within various XC approximations / Effects of Carbon Nanotube Oxidation on Molecular Interactions. Materials Research Society Symposia Proceedings, 2008, 1084, 50301.	0.1	0
70	Electronic and optical properties of polypyridylruthenium derivatized polystyrenes: multi-level computational analysis of metallo-polymeric chromophore assemblies. Physical Chemistry Chemical Physics, 2015, 17, 1776-1784.	1.3	0