Yosuke Kanai

List of Publications by Year
in descending order

70 papers	2,271 citations	201674 27 h-index	223800 46 g-index
75 all docs	75 docs citations	75 times ranked	2997 citing authors

#	Article	IF	Citations
1	First Principles Dynamics Study of Excited Hole Relaxation in DNA. ChemPhysChem, 2022, 23, .	2.1	2
2	Nonlinear electronic excitation in water under proton irradiation: a first principles study. Physical Chemistry Chemical Physics, 2022, 24, 5598-5603.	2.8	3
3	All-Electron BSE@GW Method for K-Edge Core Electron Excitation Energies. Journal of Chemical Theory and Computation, 2022, 18, 1569-1583.	5.3	20
4	Nuclearâ€“electronic orbital approach to quantization of protons in periodic electronic structure calculations. Journal of Chemical Physics, 2022, 156, .	3.0	3
5	Dynamical transition orbitals: A particleâ€“hole description in real-time TDDFT dynamics. Journal of Chemical Physics, 2021, 154, 054107.	3.0	11
6	First-Principles Demonstration of Nonadiabatic Thouless Pumping of Electrons in a Molecular System. Journal of Physical Chemistry Letters, 2021, 12, 4496-4503.	4.6	4
7	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.	4.6	16
8	Simulating electronic excitation and dynamics with real-time propagation approach to TDDFT within plane-wave pseudopotential formulation. Journal of Chemical Physics, 2021, 155, 100901.	3.0	24
9	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.	3.0	14
10	First-Principles Modeling of Electronic Stopping in Complex Matter under Ion Irradiation. Journal of Physical Chemistry Letters, 2020, 11, 229-237.	4.6	13
11	Enabling Aqueous NiO Photocathodes by Passivating Surface Sites That Facilitate Proton-Coupled Charge Transfer. ACS Applied Energy Materials, 2020, 3, 10702-10713.	5.1	10
12	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.	3.0	22
13	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.	3.0	38
14	<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.	7.8	34
15	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.	7.1	10
16	Propagation of maximally localized Wannier functions in real-time TDDFT. Journal of Chemical Physics, 2019, 150, 194113.	3.0	20
17	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.	3.1	4
18	Electronic Excitation Dynamics in DNA under Proton and Î±-Particle Irradiation. Journal of the American Chemical Society, 2019, 141, 5241-5251.	13.7	27

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19	Dependence of hot electron transfer on surface coverage and adsorbate species at semiconductorâ€“molecule interfaces. Physical Chemistry Chemical Physics, 2018, 20, 12986-12991.	2.8	6
20	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.	5.3	41
21	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.	3.1	20
22	Tunable Semiconductors: Control over Carrier States and Excitations in Layered Hybrid Organic-Inorganic Perovskites. Physical Review Letters, 2018, 121, 146401.	7.8	103
23	Modeling Plasmon-Induced Hot-Carrier Transfer. CheM, 2018, 4, 937-939.	11.7	1
24	Electronic Excitation Dynamics in Liquid Water under Proton Irradiation. Scientific Reports, 2017, 7, 40379.	3.3	18
25	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.	5.3	15
26	Examining real-time time-dependent density functional theory nonequilibrium simulations for the calculation of electronic stopping power. Physical Review B, 2017, 96, .	3.2	60
27	Plane-wave pseudopotential implementation and performance of SCAN meta-GGA exchange-correlation functional for extended systems. Journal of Chemical Physics, 2017, 146, 224105.	3.0	66
28	Diffusion quantum Monte Carlo study of martensitic phase transition energetics: The case of phosphorene. Journal of Chemical Physics, 2016, 145, 124705.	3.0	7
29	Excited Electron Dynamics at Semiconductorâ€“Molecule Type-II Heterojunction Interface: First-Principles Dynamics Simulation. Journal of Physical Chemistry Letters, 2016, 7, 1495-1500.	4.6	17
30	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, .	3.2	37
31	Electronic stopping power in liquid water for protons and Î± particles from first principles. Physical Review B, 2016, 94, .	3.2	46
32	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.	3.1	44
33	Site-Selective Passivation of Defects in NiO Solar Photocathodes by Targeted Atomic Deposition. ACS Applied Materials & Interfaces, 2016, 8, 4754-4761.	8.0	71
34	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, .	3.2	22
35	Communication: Modeling of concentration dependent water diffusivity in ionic solutions: Role of intermolecular charge transfer. Journal of Chemical Physics, 2015, 143, 241101.	3.0	53
36	Accurate atomistic first-principles calculations of electronic stopping. Physical Review B, 2015, 91, .	3.2	121

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37	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.	2.8	0
38	Role of Surface Termination on Hot Electron Relaxation in Silicon Quantum Dots: A First-Principles Dynamics Simulation Study. Nano Letters, 2015, 15, 6429-6433.	9.1	73
39	Reptation Quantum Monte Carlo calculation of charge transfer: The Naâ€“Cl dimer. Chemical Physics Letters, 2015, 618, 236-240.	2.6	4
40	Quantum Dynamics Simulation of Electrons in Materials on High-Performance Computers. Computing in Science and Engineering, 2014, 16, 54-60.	1.2	41
41	Scaling and spatial analysis of the dielectric response of cadmium selenide nanowires. Physical Review B, 2014, 90, .	3.2	1
42	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.	3.0	11
43	Modeling time-coincident ultrafast electron transfer and solvation processes at molecule-semiconductor interfaces. Journal of Chemical Physics, 2014, 140, 234109.	3.0	5
44	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.	3.3	35
45	Importance of Excitonic Effect in Charge Separation at Quantum-Dot/Organic Interface: First-Principles Many-Body Calculations. Nano Letters, 2014, 14, 6884-6888.	9.1	8
46	Role of Charge Transfer in Water Diffusivity in Aqueous Ionic Solutions. Journal of Physical Chemistry Letters, 2014, 5, 2711-2716.	4.6	46
47	Dependence of Water Dynamics on Molecular Adsorbates near Hydrophobic Surfaces: First-Principles Molecular Dynamics Study. Journal of Physical Chemistry C, 2014, 118, 8508-8513.	3.1	9
48	Atom Transfer Radical Polymerization Preparation and Photophysical Properties of Polypyridylruthenium Derivatized Polystyrenes. Inorganic Chemistry, 2013, 52, 8511-8520.	4.0	21
49	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.	13.7	41
50	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.	4.6	15
51	Plane-wave pseudopotential implementation of explicit integrators for time-dependent Kohn-Sham equations in large-scale simulations. Journal of Chemical Physics, 2012, 137, 22A546.	3.0	80
52	Xâ€ray Transient Absorption and Picosecond IR Spectroscopy of Fulvalene(tetracarbonyl)diruthenium on Photoexcitation. Angewandte Chemie - International Edition, 2012, 51, 7692-7696.	13.8	47
53	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.	3.1	2
54	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.	14.6	16

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55	Theory and Simulation of Nanostructured Materials for Photovoltaic Applications. Computing in Science and Engineering, 2010, 12, 18-27.	1.2	7
56	Mechanism of Thermal Reversal of the (Fulvalene)tetracarbonyldiruthenium Photoisomerization: Toward Molecular Solarâ€“Thermal Energy Storage. Angewandte Chemie - International Edition, 2010, 49, 8926-8929.	13.8	105
57	Atomistic Oxidation Mechanism of a Carbon Nanotube in Nitric Acid. Physical Review Letters, 2010, 104, 066401.	7.8	52
58	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.	3.1	22
59	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
60	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.	3.0	16
61	Quantum Monte Carlo calculations of the energy-level alignment at hybrid interfaces: Role of many-body effects. Physical Review B, 2009, 79, .	3.2	12
62	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, .	2.5	21
63	Role of Semiconducting and Metallic Tubes in P3HT/Carbon-Nanotube Photovoltaic Heterojunctions: Density Functional Theory Calculations. Nano Letters, 2008, 8, 908-912.	9.1	145
64	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
65	Insights on Interfacial Charge Transfer Across P3HT/Fullerene Photovoltaic Heterojunction from Ab Initio Calculations. Nano Letters, 2007, 7, 1967-1972.	9.1	136
66	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.	3.0	46
67	Competing Mechanisms in the Optically Activated Functionalization of the Hydrogen-Terminated Si(111) Surface. Journal of the American Chemical Society, 2006, 128, 3892-3893.	13.7	24
68	A Theoretical Study of Biotin Chemisorption on Siâˆ’SiC(001) Surfaces. Journal of Physical Chemistry B, 2005, 109, 13656-13662.	2.6	20
69	Role of Molecular Conjugation in the Surface Radical Reaction of Aldehydes with Hâˆ’Si(111):â€‰ First Principles Study. Journal of Physical Chemistry B, 2005, 109, 18889-18894.	2.6	31
70	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.	13.7	86