

# Yosuke Kanai

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/3506426/publications.pdf>

Version: 2024-02-01

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	First Principles Dynamics Study of Excited Hole Relaxation in DNA. ChemPhysChem, 2022, 23, .	1.0	2
2	Nonlinear electronic excitation in water under proton irradiation: a first principles study. Physical Chemistry Chemical Physics, 2022, 24, 5598-5603.	1.3	3
3	All-Electron BSE@ <i>GW</i> Method for <i>K</i> -Edge Core Electron Excitation Energies. Journal of Chemical Theory and Computation, 2022, 18, 1569-1583.	2.3	20
4	Nuclearâ€“electronic orbital approach to quantization of protons in periodic electronic structure calculations. Journal of Chemical Physics, 2022, 156, .	1.2	3
5	Dynamical transition orbitals: A particleâ€“hole description in real-time TDDFT dynamics. Journal of Chemical Physics, 2021, 154, 054107.	1.2	11
6	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
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.	2.1	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.	1.2	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.	1.2	14
10	First-Principles Modeling of Electronic Stopping in Complex Matter under Ion Irradiation. Journal of Physical Chemistry Letters, 2020, 11, 229-237.	2.1	13
11	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
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.	1.2	22
13	All-electron <i>ab initio</i> Bethe-Salpeter equation approach to neutral excitations in molecules with numeric atom-centered orbitals. Journal of Chemical Physics, 2020, 152, 044105.	1.2	38
14	$\langle \text{Shell Core-Electron Excitations in Electronic Stopping of Protons in Water from First Principles. Physical Review Letters, 2019, 123, 066401.} \rangle$	2.9	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.	3.3	10
16	Propagation of maximally localized Wannier functions in real-time TDDFT. Journal of Chemical Physics, 2019, 150, 194113.	1.2	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.	1.5	4
18	Electronic Excitation Dynamics in DNA under Proton and $\hat{\pm}$ -Particle Irradiation. Journal of the American Chemical Society, 2019, 141, 5241-5251.	6.6	27

#	ARTICLE	IF	CITATIONS
19	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.	1.3	6
20	Free Energy Profile of NaCl in Water: First-Principles Molecular Dynamics with SCAN and $\gamma$ -B97X-V Exchange–Correlation Functionals. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 884-893.	2.3	41
21	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.	1.5	20
22	Tunable Semiconductors: Control over Carrier States and Excitations in Layered Hybrid Organic-Inorganic Perovskites. <i>Physical Review Letters</i> , 2018, 121, 146401.	2.9	103
23	Modeling Plasmon-Induced Hot-Carrier Transfer. <i>CheM</i> , 2018, 4, 937-939.	5.8	1
24	Electronic Excitation Dynamics in Liquid Water under Proton Irradiation. <i>Scientific Reports</i> , 2017, 7, 40379.	1.6	18
25	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.	2.3	15
26	Examining real-time time-dependent density functional theory nonequilibrium simulations for the calculation of electronic stopping power. <i>Physical Review B</i> , 2017, 96, .	1.1	60
27	Plane-wave pseudopotential implementation and performance of SCAN meta-GGA exchange–correlation functional for extended systems. <i>Journal of Chemical Physics</i> , 2017, 146, 224105.	1.2	66
28	Diffusion quantum Monte Carlo study of martensitic phase transition energetics: The case of phosphorene. <i>Journal of Chemical Physics</i> , 2016, 145, 124705.	1.2	7
29	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.	2.1	17
30	Electronic stopping for protons and $\hat{\pm}$ particles from first-principles electron dynamics: The case of silicon carbide. <i>Physical Review B</i> , 2016, 94, .	1.1	37
31	Electronic stopping power in liquid water for protons and $\hat{\pm}$ particles from first principles. <i>Physical Review B</i> , 2016, 94, .	1.1	46
32	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.	1.5	44
33	Site-Selective Passivation of Defects in NiO Solar Photocathodes by Targeted Atomic Deposition. <i>ACS Applied Materials &amp; Interfaces</i> , 2016, 8, 4754-4761.	4.0	71
34	Antiferromagnetic structures and electronic energy levels at reconstructed NiO(111) surfaces: A $\gamma$ -B97X-V DFT study. <i>Physical Review B</i> , 2015, 91, .	1.1	22
35	Communication: Modeling of concentration dependent water diffusivity in ionic solutions: Role of intermolecular charge transfer. <i>Journal of Chemical Physics</i> , 2015, 143, 241101.	1.2	53
36	Accurate atomistic first-principles calculations of electronic stopping. <i>Physical Review B</i> , 2015, 91, .	1.1	121

#	ARTICLE	IF	CITATIONS
37	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.	1.3	0
38	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.	4.5	73
39	Reptation Quantum Monte Carlo calculation of charge transfer: The Na <sup>+</sup> Cl <sup>-</sup> dimer. <i>Chemical Physics Letters</i> , 2015, 618, 236-240.	1.2	4
40	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
41	Scaling and spatial analysis of the dielectric response of cadmium selenide nanowires. <i>Physical Review B</i> , 2014, 90, .	1.1	1
42	Theoretical oxidation state analysis of Ru-(bpy) <sub>3</sub> : Influence of water solvation and Hubbard correction in first-principles calculations. <i>Journal of Chemical Physics</i> , 2014, 141, 024305.	1.2	11
43	Modeling time-coincident ultrafast electron transfer and solvation processes at molecule-semiconductor interfaces. <i>Journal of Chemical Physics</i> , 2014, 140, 234109.	1.2	5
44	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.	1.7	35
45	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.	4.5	8
46	Role of Charge Transfer in Water Diffusivity in Aqueous Ionic Solutions. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 2711-2716.	2.1	46
47	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.	1.5	9
48	Atom Transfer Radical Polymerization Preparation and Photophysical Properties of Polypyridylruthenium Derivatized Polystyrenes. <i>Inorganic Chemistry</i> , 2013, 52, 8511-8520.	1.9	21
49	Role of Four-Fold Coordinated Titanium and Quantum Confinement in CO <sub>2</sub> Reduction at Titania Surface. <i>Journal of the American Chemical Society</i> , 2012, 134, 20266-20269.	6.6	41
50	Biomimetic Carbon Nanotube for Catalytic CO <sub>2</sub> 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.	2.1	15
51	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.	1.2	80
52	X-ray Transient Absorption and Picosecond IR Spectroscopy of Fulvalene(tetracarbonyl)diruthenium on Photoexcitation. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 7692-7696.	7.2	47
53	Cooperative Chiral Adsorption of Styrene Molecules on the Si(001)-(2 × 4) Surface: First-Principles Investigation of Reaction Mechanisms. <i>Journal of Physical Chemistry C</i> , 2011, 115, 14213-14218.	1.5	2
54	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.	7.3	16

#	ARTICLE	IF	CITATIONS
55	Theory and Simulation of Nanostructured Materials for Photovoltaic Applications. <i>Computing in Science and Engineering</i> , 2010, 12, 18-27.	1.2	7
56	Mechanism of Thermal Reversal of the (Fulvalene)tetracarbonyliruthenium Photoisomerization: Toward Molecular Solar- $\epsilon$ Thermal Energy Storage. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 8926-8929.	7.2	105
57	Atomistic Oxidation Mechanism of a Carbon Nanotube in Nitric Acid. <i>Physical Review Letters</i> , 2010, 104, 066401.	2.9	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. <i>Journal of Physical Chemistry C</i> , 2010, 114, 3981-3986.	1.5	22
59	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
60	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.	1.2	16
61	Quantum Monte Carlo calculations of the energy-level alignment at hybrid interfaces: Role of many-body effects. <i>Physical Review B</i> , 2009, 79, .	1.1	12
62	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, .	1.0	21
63	Role of Semiconducting and Metallic Tubes in P3HT/Carbon-Nanotube Photovoltaic Heterojunctions: Density Functional Theory Calculations. <i>Nano Letters</i> , 2008, 8, 908-912.	4.5	145
64	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
65	Insights on Interfacial Charge Transfer Across P3HT/Fullerene Photovoltaic Heterojunction from Ab Initio Calculations. <i>Nano Letters</i> , 2007, 7, 1967-1972.	4.5	136
66	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.	1.2	46
67	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.	6.6	24
68	A Theoretical Study of Biotin Chemisorption on Si $\epsilon$ -SiC(001) Surfaces. <i>Journal of Physical Chemistry B</i> , 2005, 109, 13656-13662.	1.2	20
69	Role of Molecular Conjugation in the Surface Radical Reaction of Aldehydes with H $\epsilon$ -Si(111): $\epsilon$ First Principles Study. <i>Journal of Physical Chemistry B</i> , 2005, 109, 18889-18894.	1.2	31
70	Surface Reaction of Alkynes and Alkenes with H-Si(111): $\epsilon$ A Density Functional Theory Study. <i>Journal of the American Chemical Society</i> , 2004, 126, 15890-15896.	6.6	86