Alexey V Akimov

List of Publications by Year
in descending order

67	4,241	159525 30	110317 64
papers	citations	h-index	g-index

69	69	69	3085
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The PYXAID Program for Non-Adiabatic Molecular Dynamics in Condensed Matter Systems. Journal of Chemical Theory and Computation, 2013, 9, 4959-4972.	2.3	588
2	Advanced Capabilities of the PYXAID Program: Integration Schemes, Decoherence Effects, Multiexcitonic States, and Field-Matter Interaction. Journal of Chemical Theory and Computation, 2014, 10, 789-804.	2.3	472
3	Theoretical Insights into Photoinduced Charge Transfer and Catalysis at Oxide Interfaces. Chemical Reviews, 2013, 113, 4496-4565.	23.0	455
4	Recent Progress in Surface Hopping: 2011â€“2015. Journal of Physical Chemistry Letters, 2016, 7, 2100-2112.	2.1	279
5	Large-Scale Computations in Chemistry: A Birdâ€™s Eye View of a Vibrant Field. Chemical Reviews, 2015, 115, 5797-5890.	23.0	182
6	Persistent Electronic Coherence Despite Rapid Loss of Electronâ€“Nuclear Correlation. Journal of Physical Chemistry Letters, 2013, 4, 3857-3864.	2.1	165
7	Nonadiabatic Dynamics of Charge Transfer and Singlet Fission at the Pentacene/C₆₀ Interface. Journal of the American Chemical Society, 2014, 136, 1599-1608.	6.6	142
8	Spinâ€“Orbit Interactions Greatly Accelerate Nonradiative Dynamics in Lead Halide Perovskites. ACS Energy Letters, 2018, 3, 2159-2166.	8.8	114
9	Nonadiabatic Dynamics of Positive Charge during Photocatalytic Water Splitting on GaN(10-10) Surface: Charge Localization Governs Splitting Efficiency. Journal of the American Chemical Society, 2013, 135, 8682-8691.	6.6	107
10	What Makes the Photocatalytic CO₂ Reduction on N-Doped Ta₂O₅ Efficient: Insights from Nonadiabatic Molecular Dynamics. Journal of the American Chemical Society, 2015, 137, 11517-11525.	6.6	105
11	Nonradiative Electronâ€“Hole Recombination Rate Is Greatly Reduced by Defects in Monolayer Black Phosphorus: Ab Initio Time Domain Study. Journal of Physical Chemistry Letters, 2016, 7, 653-659.	2.1	99
12	Cation Effect on Hot Carrier Cooling in Halide Perovskite Materials. Journal of Physical Chemistry Letters, 2017, 8, 4439-4445.	2.1	97
13	Nonadiabatic Molecular Dynamics for Thousand Atom Systems: A Tight-Binding Approach toward PYXAID. Journal of Chemical Theory and Computation, 2016, 12, 1436-1448.	2.3	93
14	Coherence penalty functional: A simple method for adding decoherence in Ehrenfest dynamics. Journal of Chemical Physics, 2014, 140, 194107.	1.2	86
15	Molecular Dynamics of Surface-Moving Thermally Driven Nanocars. Journal of Chemical Theory and Computation, 2008, 4, 652-656.	2.3	81
16	Libra: An open-Source â€œmethodology discoveryâ€•library for quantum and classical dynamics simulations. Journal of Computational Chemistry, 2016, 37, 1626-1649.	1.5	71
17	Accurate Computation of Nonadiabatic Coupling with Projector Augmented-Wave Pseudopotentials. Journal of Physical Chemistry Letters, 2020, 11, 10073-10080.	2.1	65
18	A Simple Phase Correction Makes a Big Difference in Nonadiabatic Molecular Dynamics. Journal of Physical Chemistry Letters, 2018, 9, 6096-6102.	2.1	64

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19	Enhancing the carrier thermalization time in organometallic perovskites by halide mixing. Physical Chemistry Chemical Physics, 2016, 18, 5219-5231.	1.3	61
20	Theoretical Investigation of Electron and Nuclear Dynamics in the [Au₂₅(SH)₁₈]^{â^'1} Thiolate-Protected Gold Nanocluster. Journal of Physical Chemistry C, 2017, 121, 10653-10662.	1.5	48
21	Modeling nonadiabatic dynamics in condensed matter materials: some recent advances and applications. Journal of Physics Condensed Matter, 2020, 32, 073001.	0.7	45
22	Unidirectional Rolling Motion of Nanocars Induced by Electric Field. Journal of Physical Chemistry C, 2012, 116, 22595-22601.	1.5	44
23	Criticality of Symmetry in Rational Design of Chalcogenide Perovskites. Journal of Physical Chemistry Letters, 2018, 9, 248-257.	2.1	43
24	Dependence of Nonadiabatic Couplings with Kohnâ€“Sham Orbitals on the Choice of Density Functional: Pure vs Hybrid. Journal of Physical Chemistry A, 2016, 120, 9028-9041.	1.1	39
25	Rigid-Body Molecular Dynamics of Fullerene-Based Nanocars on Metallic Surfaces. Journal of Chemical Theory and Computation, 2010, 6, 2581-2590.	2.3	38
26	Charge Transfer and Chemisorption of Fullerene Molecules on Metal Surfaces: Application to Dynamics of Nanocars. Journal of Physical Chemistry C, 2012, 116, 13816-13826.	1.5	37
27	Nonadiabatic Molecular Dynamics with Tight-Binding Fragment Molecular Orbitals. Journal of Chemical Theory and Computation, 2016, 12, 5719-5736.	2.3	36
28	Dynamics of Thioether Molecular Rotors: Effects of Surface Interactions and Chain Flexibility. Journal of Physical Chemistry C, 2009, 113, 10913-10920.	1.5	33
29	Second-Quantized Surface Hopping. Physical Review Letters, 2014, 113, 153003.	2.9	33
30	Excited-State Dynamics in Two-Dimensional Heterostructures: SiR/TiO₂ and GeR/TiO₂ (R = H, Me) as Promising Photocatalysts. Journal of Physical Chemistry C, 2017, 121, 6520-6532.	1.5	33
31	Non-adiabatic molecular dynamics with Î”SCF excited states. Journal of Physics Condensed Matter, 2018, 30, 484002.	0.7	30
32	Upward Shift in Conduction Band of Ta2O5 Due to Surface Dipoles Induced by N-Doping. Journal of Physical Chemistry C, 2015, 119, 26925-26936.	1.5	27
33	Quantized Hamiltonian dynamics captures the low-temperature regime of charge transport in molecular crystals. Journal of Chemical Physics, 2013, 139, 174109.	1.2	25
34	A comparative analysis of surface hopping acceptance and decoherence algorithms within the neglect of back-reaction approximation. Journal of Chemical Physics, 2019, 151, 124107.	1.2	24
35	Molecular Dynamics Study of Crystalline Molecular Gyroscopes. Journal of Physical Chemistry C, 2011, 115, 13584-13591.	1.5	23
36	Nonadiabatic Dynamics in Si and CdSe Nanoclusters: Many-Body vs Single-Particle Treatment of Excited States. Journal of Chemical Theory and Computation, 2021, 17, 678-693.	2.3	22

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37	Spinâ€“Orbit Coupling Accelerates the Photoinduced Interfacial Electron Transfer in a Fullerene-Based Perovskite Heterojunction. Journal of Physical Chemistry Letters, 2021, 12, 1131-1137.	2.1	21
38	Theoretical Insights into the Impact of Ru Catalyst Anchors on the Efficiency of Photocatalytic CO₂ Reduction on Ta₂O₅. Journal of Physical Chemistry B, 2015, 119, 7186-7197.	1.2	20
39	Charge transfer dynamics at the boron subphthalocyanine chloride/C₆₀ interface: non-adiabatic dynamics study with Libra-X. Physical Chemistry Chemical Physics, 2018, 20, 25275-25294.	1.3	20
40	Role of Graphene Surface Ripples and Thermal Vibrations in Molecular Dynamics of C₆₀. Journal of Physical Chemistry C, 2019, 123, 20026-20036.	1.5	19
41	Hot Electron Cooling in Silicon Nanoclusters via Landauâ€“Zener Nonadiabatic Molecular Dynamics: Size Dependence and Role of Surface Termination. Journal of Physical Chemistry Letters, 2020, 11, 1456-1465.	2.1	19
42	Supersymmetry and fluctuation relations for currents in closed networks. Physical Review E, 2011, 83, 021107.	0.8	18
43	Analysis of the Trajectory Surface Hopping Method from the Markov State Model Perspective. Journal of the Physical Society of Japan, 2015, 84, 094002.	0.7	17
44	Dynamics of Single-Molecule Rotations on Surfaces that Depend on Symmetry, Interactions, and Molecular Sizes. Journal of Physical Chemistry C, 2011, 115, 125-131.	1.5	16
45	Persistent Quantum Coherence and Strong Coupling Enable Fast Electron Transfer across the CdS/TiO₂ Interface: A Time-Domain ab Initio Simulation. Journal of Physical Chemistry C, 2018, 122, 25606-25616.	1.5	16
46	Extending the Time Scales of Nonadiabatic Molecular Dynamics via Machine Learning in the Time Domain. Journal of Physical Chemistry Letters, 2021, 12, 12119-12128.	2.1	16
47	Formulation of quantized Hamiltonian dynamics in terms of natural variables. Journal of Chemical Physics, 2012, 137, 224115.	1.2	14
48	Scaling relationships for nonadiabatic energy relaxation times in warm dense matter: toward understanding the equation of state. Physical Chemistry Chemical Physics, 2016, 18, 32466-32476.	1.3	14
49	Locomotion of the C60-based nanomachines on graphene surfaces. Scientific Reports, 2021, 11, 2576.	1.6	13
50	Crystal Symmetry and Static Electron Correlation Greatly Accelerate Nonradiative Dynamics in Lead Halide Perovskites. Journal of Physical Chemistry Letters, 2021, 12, 2444-2453.	2.1	13
51	Excited state dynamics in monolayer black phosphorus revisited: Accounting for many-body effects. Journal of Chemical Physics, 2021, 155, 134106.	1.2	13
52	Stochastic and Quasi-Stochastic Hamiltonians for Long-Time Nonadiabatic Molecular Dynamics. Journal of Physical Chemistry Letters, 2017, 8, 5190-5195.	2.1	12
53	Recursive Taylor Series Expansion Method for Rigid-Body Molecular Dynamics. Journal of Chemical Theory and Computation, 2011, 7, 3062-3071.	2.3	10
54	Dependence of electron transfer dynamics on the number of graphene layers in Ï€-stacked 2D materials: insights from ab initio nonadiabatic molecular dynamics. Physical Chemistry Chemical Physics, 2019, 21, 23198-23208.	1.3	10

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55	Analysis of self-consistent extended HÃ¼ckel theory (SC-EHT): a new look at the old method. Journal of Mathematical Chemistry, 2015, 53, 528-550.	0.7	9
56	A Simple Solution to Trivial Crossings: A Stochastic State Tracking Approach. Journal of Physical Chemistry Letters, 2021, 12, 850-860.	2.1	8
57	Nonadiabatic Molecular Dynamics with Extended Density Functional Tight-Binding: Application to Nanocrystals and Periodic Solids. Journal of Chemical Theory and Computation, 2022, 18, 5157-5180.	2.3	6
58	Sensitivity field for nonautonomous molecular rotors. Journal of Chemical Physics, 2011, 135, 224104.	1.2	5
59	Hierarchical equations of motion in the Libra software package. International Journal of Quantum Chemistry, 2020, 120, e26373.	1.0	5
60	Directed motion of periodically driven molecular motors: A graph-theoretical approach. Journal of Chemical Physics, 2013, 138, 024109.	1.2	4
61	Theory of solar energy materials. Journal of Physics Condensed Matter, 2015, 27, 130301.	0.7	3
62	Nonradiative Relaxation of Charge Carriers in GaN-InN Alloys: Insights from Nonadiabatic Molecular Dynamics. ACS Symposium Series, 2015, , 189-200.	0.5	3
63	Entangled trajectories Hamiltonian dynamics for treating quantum nuclear effects. Journal of Chemical Physics, 2018, 148, 144106.	1.2	3
64	Theory of Nonadiabatic Electron Dynamics in Nanomaterials. , 2015, , 1-20.		3
65	Implementation of a molecular dynamics approach with rigid fragments to simulation of chemical reactions in biomolecular systems. Moscow University Chemistry Bulletin, 2007, 62, 177-179.	0.2	2
66	Analysis of depolarization ratios of ClNO2 dissolved in methanol. Journal of Chemical Physics, 2014, 140, 014301.	1.2	1
67	Theory of Nonadiabatic Electron Dynamics in Nanomaterials. , 2016, , 4086-4103.		0