Oleg Prezhdo

List of Publications by Citations

455 papers	20,306 citations	81 h-index	122 g-index
495 ext. papers	22,763 ext. citations	7.5 avg, IF	7.73 L-index

#	Paper	IF	Citations
455	Trajectory surface hopping in the time-dependent Kohn-Sham approach for electron-nuclear dynamics. *Physical Review Letters*, **2005**, 95, 163001	7.4	505
454	Theoretical studies of photoinduced electron transfer in dye-sensitized TiO2. *Annual Review of Physical Chemistry*, **2007**, 58, 143-84	15.7	487
453	The PYXAID Program for Non-Adiabatic Molecular Dynamics in Condensed Matter Systems. *Journal of Chemical Theory and Computation*, **2013**, 9, 4959-72	6.4	413
452	Theoretical insights into photoinduced charge transfer and catalysis at oxide interfaces. *Chemical Reviews*, **2013**, 113, 4496-565	68.1	392
451	Decoherence-induced surface hopping. *Journal of Chemical Physics*, **2012**, 137, 22A545	3.9	370
450	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	6.4	332
449	Quantum decoherence and the isotope effect in condensed phase nonadiabatic molecular dynamics simulations. *Journal of Chemical Physics*, **1996**, 104, 5942-5955	3.9	299
448	Mean-field molecular dynamics with surface hopping. *Journal of Chemical Physics*, **1997**, 107, 825-834	3.9	286
447	Unravelling the Effects of Grain Boundary and Chemical Doping on Electron-Hole Recombination in CH3NH3PbI3 Perovskite by Time-Domain Atomistic Simulation. *Journal of the American Chemical Society*, **2016**, 138, 3884-90	16.4	272
446	Evaluation of quantum transition rates from quantum-classical molecular dynamics simulations. *Journal of Chemical Physics*, **1997**, 107, 5863-5878	3.9	256
445	Ab initio nonadiabatic molecular dynamics of the ultrafast electron injection across the alizarin-TiO2 interface. *Journal of the American Chemical Society*, **2005**, 127, 7941-51	16.4	242
444	Detection of nucleic acids with graphene nanopores: ab initio characterization of a novel sequencing device. *Nano Letters*, **2010**, 10, 3237-42	11.5	222
443	Photo-induced charge separation across the graphene-TiO2 interface is faster than energy losses: a time-domain ab initio analysis. *Journal of the American Chemical Society*, **2012**, 134, 14238-48	16.4	206
442	Breaking the phonon bottleneck in PbSe and CdSe quantum dots: time-domain density functional theory of charge carrier relaxation. *ACS Nano*, **2009**, 3, 93-9	16.7	206
441	Recent Progress in Surface Hopping: 2011-2015. *Journal of Physical Chemistry Letters*, **2016**, 7, 2100-12	6.4	200
440	Ultrafast carrier thermalization and cooling dynamics in few-layer MoS2. *ACS Nano*, **2014**, 8, 10931-40	16.7	192
439	Time-domain ab initio study of charge relaxation and recombination in dye-sensitized TiO2. *Journal of the American Chemical Society*, **2007**, 129, 8528-43	16.4	192

438	Shape-controlled synthesis of silver nanoparticles: Ab initio study of preferential surface coordination with citric acid. *Chemical Physics Letters*, **2008**, 458, 113-116	2.5	182
437	Quantum Zeno effect rationalizes the phonon bottleneck in semiconductor quantum dots. *Physical Review Letters*, **2013**, 110, 180404	7.4	181
436	Instantaneous generation of charge-separated state on TiO surface sensitized with plasmonic nanoparticles. *Journal of the American Chemical Society*, **2014**, 136, 4343-54	16.4	180
435	Electronic structure and spectra of catechol and alizarin in the gas phase and attached to titanium. *Journal of Physical Chemistry B*, **2005**, 109, 365-73	3.4	178
434	Mixing quantum and classical mechanics. *Physical Review A*, **1997**, 56, 162-175	2.6	172
433	Quantum Coherence Facilitates Efficient Charge Separation at a MoS2/MoSe2 van der Waals Junction. *Nano Letters*, **2016**, 16, 1996-2003	11.5	170
432	Colloidal semiconductor quantum dots with tunable surface composition. *Nano Letters*, **2012**, 12, 4465-71	11.5	165
431	Nonadiabatic Molecular Dynamics Simulation of Light-Induced Electron Transfer from an Anchored Molecular Electron Donor to a Semiconductor Acceptor. *Journal of Physical Chemistry B*, **2002**, 106, 8047-8054	3.4	165
430	Relationship between Quantum Decoherence Times and Solvation Dynamics in Condensed Phase Chemical Systems. *Physical Review Letters*, **1998**, 81, 5294-5297	7.4	162
429	Auger-assisted electron transfer from photoexcited semiconductor quantum dots. *Nano Letters*, **2014**, 14, 1263-9	11.5	160
428	Photoinduced electron dynamics at the chromophore semiconductor interface: A time-domain ab initio perspective. *Progress in Surface Science*, **2009**, 84, 30-68	6.6	155
427	Large-Scale Computations in Chemistry: A Bird's Eye View of a Vibrant Field. *Chemical Reviews*, **2015**, 115, 5797-890	68.1	152
426	Regarding the validity of the time-dependent Kohn-Sham approach for electron-nuclear dynamics via trajectory surface hopping. *Journal of Chemical Physics*, **2011**, 134, 024102	3.9	149
425	The two-pathway model for the catch-slip transition in biological adhesion. *Biophysical Journal*, **2005**, 89, 1446-54	2.9	149
424	Quantum backreaction through the Bohmian particle. *Physical Review Letters*, **2001**, 86, 3215-9	7.4	140
423	Mean field approximation for the stochastic Schrdinger equation. *Journal of Chemical Physics*, **1999**, 111, 8366-8377	3.9	137
422	A Simple Solution to the Trivial Crossing Problem in Surface Hopping. *Journal of Physical Chemistry Letters*, **2014**, 5, 713-9	6.4	129
421	Persistent Electronic Coherence Despite Rapid Loss of Electron Nuclear Correlation. *Journal of Physical Chemistry Letters*, **2013**, 4, 3857-3864	6.4	128

420	Acetonitrile boosts conductivity of imidazolium ionic liquids. *Journal of Physical Chemistry B*, **2012**, 116, 7719-27	3.4	123
419	Scanning tunneling microscopy of DNA-wrapped carbon nanotubes. *Nano Letters*, **2009**, 9, 12-7	11.5	121
418	Phonon-Assisted Ultrafast Charge Transfer at van der Waals Heterostructure Interface. *Nano Letters*, **2017**, 17, 6435-6442	11.5	120
417	Dynamics of the photoexcited electron at the chromophore-semiconductor interface. *Accounts of Chemical Research*, **2008**, 41, 339-48	24.3	118
416	Nonadiabatic dynamics of charge transfer and singlet fission at the pentacene/C60 interface. *Journal of the American Chemical Society*, **2014**, 136, 1599-608	16.4	115
415	Nonradiative quenching of fluorescence in a semiconducting carbon nanotube: a time-domain ab initio study. *Physical Review Letters*, **2008**, 100, 197402	7.4	115
414	Hole Trapping by Iodine Interstitial Defects Decreases Free Carrier Losses in Perovskite Solar Cells: A Time-Domain Ab Initio Study. *ACS Energy Letters*, **2017**, 2, 1270-1278	20.1	114
413	Ab initio nonadiabatic molecular dynamics of the ultrafast electron injection from a PbSe quantum dot into the TiO2 surface. *Journal of the American Chemical Society*, **2011**, 133, 19240-9	16.4	114
412	Maximizing Singlet Fission by Intermolecular Packing. *Journal of Physical Chemistry Letters*, **2014**, 5, 3345-53	6.4	113
411	Surface ligands increase photoexcitation relaxation rates in CdSe quantum dots. *ACS Nano*, **2012**, 6, 6515-24	14.7	113
410	Moderate Humidity Delays Electron-Hole Recombination in Hybrid Organic-Inorganic Perovskites: Time-Domain Ab Initio Simulations Rationalize Experiments. *Journal of Physical Chemistry Letters*, **2016**, 7, 3215-22	6.4	109
409	Photoinduced dynamics in semiconductor quantum dots: insights from time-domain ab initio studies. *Accounts of Chemical Research*, **2009**, 42, 2005-16	24.3	108
408	Guest–Host Cooperativity in Organic Materials Greatly Enhances the Nonlinear Optical Response. *Journal of Physical Chemistry C*, **2008**, 112, 4355-4363	3.8	105
407	Dopants Control Electron-Hole Recombination at Perovskite-TiO$_2$ Interfaces: Ab Initio Time-Domain Study. *ACS Nano*, **2015**, 9, 11143-55	16.7	103
406	Time-domain ab initio modeling of photoinduced dynamics at nanoscale interfaces. *Annual Review of Physical Chemistry*, **2015**, 66, 549-79	15.7	103
405	Quantum anti-zeno acceleration of a chemical reaction. *Physical Review Letters*, **2000**, 85, 4413-7	7.4	103
404	Control of Charge Carriers Trapping and Relaxation in Hematite by Oxygen Vacancy Charge: Ab Initio Non-adiabatic Molecular Dynamics. *Journal of the American Chemical Society*, **2017**, 139, 6707-6717	16.4	101
403	Phonon-induced dephasing of excitons in semiconductor quantum dots: multiple exciton generation, fission, and luminescence. *ACS Nano*, **2009**, 3, 2487-94	16.7	101

402	Ab Initio Time-Domain Study of Phonon-Assisted Relaxation of Charge Carriers in a PbSe Quantum Dot. *Journal of Physical Chemistry C*, **2007**, 111, 4871-4878	3.8	101
401	Donor-Acceptor Interaction Determines the Mechanism of Photoinduced Electron Injection from Graphene Quantum Dots into TiO: Stacking Supersedes Covalent Bonding. *Journal of the American Chemical Society*, **2017**, 139, 2619-2629	16.4	100
400	Global Flux Surface Hopping Approach for Mixed Quantum-Classical Dynamics. *Journal of Chemical Theory and Computation*, **2014**, 10, 3598-605	6.4	100
399	Low-frequency lattice phonons in halide perovskites explain high defect tolerance toward electron-hole recombination. *Science Advances*, **2020**, 6, eaaw7453	14.3	99
398	Water boiling inside carbon nanotubes: toward efficient drug release. *ACS Nano*, **2011**, 5, 5647-55	16.7	97
397	Chlorine doping reduces electron-hole recombination in lead iodide perovskites: time-domain ab initio analysis. *Journal of Physical Chemistry Letters*, **2015**, 6, 4463-9	6.4	96
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395	Quantized Hamilton dynamics. *Journal of Chemical Physics*, **2000**, 113, 6557-6565	3.9	94
394	Control of Charge Recombination in Perovskites by Oxidation State of Halide Vacancy. *Journal of the American Chemical Society*, **2018**, 140, 15753-15763	16.4	94
393	Temperature independence of the photoinduced electron injection in dye-sensitized TiO2 rationalized by ab initio time-domain density functional theory. *Journal of the American Chemical Society*, **2008**, 130, 9756-62	16.4	92
392	Sulfur Adatom and Vacancy Accelerate Charge Recombination in MoS but by Different Mechanisms: Time-Domain Ab Initio Analysis. *Nano Letters*, **2017**, 17, 7962-7967	11.5	92
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390	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, 8682-91	16.4	90
389	Generation of Multiple Excitons in PbSe and CdSe Quantum Dots by Direct Photoexcitation: First-Principles Calculations on Small PbSe and CdSe Clusters. *Journal of Physical Chemistry C*, **2008**, 112, 18291-18294	3.8	90
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386	Ionic and Molecular Liquids: Working Together for Robust Engineering. *Journal of Physical Chemistry Letters*, **2013**, 4, 1423-31	6.4	89
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384	Ab initio nonadiabatic molecular dynamics of wet-electrons on the TiO(2) surface. *Journal of the American Chemical Society*, **2009**, 131, 15483-91	16.4	88
383	Halide Composition Controls Electron-Hole Recombination in Cesium-Lead Halide Perovskite Quantum Dots: A Time Domain Ab Initio Study. *Journal of Physical Chemistry Letters*, **2018**, 9, 1872-1879	6.4	87
382	Rapid Decoherence Suppresses Charge Recombination in Multi-Layer 2D Halide Perovskites: Time-Domain Ab Initio Analysis. *Nano Letters*, **2018**, 18, 2459-2466	11.5	85
381	Time-domain ab initio study of Auger and phonon-assisted auger processes in a semiconductor quantum dot. *Nano Letters*, **2011**, 11, 1845-50	11.5	85
380	Covalent Linking Greatly Enhances Photoinduced Electron Transfer in Fullerene-Quantum Dot Nanocomposites: Time-Domain Ab Initio Study. *Journal of Physical Chemistry Letters*, **2013**, 4, 1-6	6.4	84
379	Ab initio study of vibrational dephasing of electronic excitations in semiconducting carbon nanotubes. *Nano Letters*, **2007**, 7, 3260-5	11.5	84
378	Multiple exciton generation and recombination dynamics in small Si and CdSe quantum dots: an ab initio time-domain study. *ACS Nano*, **2012**, 6, 1239-50	16.7	83
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376	Nonadiabatic Molecular Dynamics for Thousand Atom Systems: A Tight-Binding Approach toward PYXAID. *Journal of Chemical Theory and Computation*, **2016**, 12, 1436-48	6.4	82
375	Spin□Orbit Interactions Greatly Accelerate Nonradiative Dynamics in Lead Halide Perovskites. *ACS Energy Letters*, **2018**, 3, 2159-2166	20.1	82
374	Solvent Mode Participation in the Nonradiative Relaxation of the Hydrated Electron. *The Journal of Physical Chemistry*, **1996**, 100, 17094-17102		81
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367	Coherence penalty functional: a simple method for adding decoherence in Ehrenfest dynamics. *Journal of Chemical Physics*, **2014**, 140, 194107	3.9	70

366	Mixed quantum-classical dynamics for charge transport in organics. *Physical Chemistry Chemical Physics*, **2015**, 17, 12395-406	3.6	69
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363	Heat-driven release of a drug molecule from carbon nanotubes: a molecular dynamics study. *Journal of Physical Chemistry B*, **2010**, 114, 13481-6	3.4	65
362	Lewis Base Passivation of Hybrid Halide Perovskites Slows Electron-Hole Recombination: Time-Domain Ab Initio Analysis. *Journal of Physical Chemistry Letters*, **2018**, 9, 1164-1171	6.4	64
361	Interplay between Localized and Free Charge Carriers Can Explain Hot Fluorescence in the CHNHPbBr Perovskite: Time-Domain Ab Initio Analysis. *Journal of the American Chemical Society*, **2017**, 139, 17327-17333	16.4	64
360	Delocalized Impurity Phonon Induced Electron-Hole Recombination in Doped Semiconductors. *Nano Letters*, **2018**, 18, 1592-1599	11.5	63
359	Ab initio study of exciton transfer dynamics from a core–shell semiconductor quantum dot to a porphyrin-sensitizer. *Journal of Photochemistry and Photobiology A: Chemistry*, **2007**, 190, 342-351	4.7	63
358	Aromaticity indices revisited: refinement and application to certain five-membered ring heterocycles. *Tetrahedron*, **2001**, 57, 5715-5729	2.4	63
357	Strong Interaction at the Perovskite/TiO2 Interface Facilitates Ultrafast Photoinduced Charge Separation: A Nonadiabatic Molecular Dynamics Study. *Journal of Physical Chemistry C*, **2017**, 121, 3797-3806	3.8	60
356	Asymmetry in the electron and hole transfer at a polymer-carbon nanotube heterojunction. *Nano Letters*, **2014**, 14, 3335-41	11.5	59
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354	Theoretical Study of Electron–Phonon Relaxation in PbSe and CdSe Quantum Dots: Evidence for Phonon Memory. *Journal of Physical Chemistry C*, **2011**, 115, 21641-21651	3.8	58
353	Uniform diffusion of acetonitrile inside carbon nanotubes favors supercapacitor performance. *Nano Letters*, **2008**, 8, 2126-30	11.5	58
352	Influence of Defects on Excited-State Dynamics in Lead Halide Perovskites: Time-Domain ab Initio Studies. *Journal of Physical Chemistry Letters*, **2019**, 10, 3788-3804	6.4	57
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348	Synergy between Ion Migration and Charge Carrier Recombination in Metal-Halide Perovskites. *Journal of the American Chemical Society*, **2020**, 142, 3060-3068	16.4	55
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335	Auger-mediated electron relaxation is robust to deep hole traps: time-domain ab initio study of CdSe quantum dots. *Nano Letters*, **2015**, 15, 2086-91	11.5	50
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329	Microscopic structure and dynamics of LiBF4 solutions in cyclic and linear carbonates. *Journal of Physical Chemistry B*, **2011**, 115, 14563-71	3.4	47
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304	Multiple Exciton Generation in Small Si Clusters: A High-Level, Ab Initio Study. *Journal of Physical Chemistry Letters*, **2010**, 1, 232-237	6.4	37
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