Oleg Prezhdo

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Interpolating Nonadiabatic Molecular Dynamics Hamiltonian with Inverse Fast Fourier Transform.. *Journal of Physical Chemistry Letters*, **2022**, 331-338	6.4	2
454	Excited State Dynamics in Dual-Defects Modified Graphitic Carbon Nitride.. *Journal of Physical Chemistry Letters*, **2022**, 1033-1041	6.4	5
453	Dimensionality reduction in machine learning for nonadiabatic molecular dynamics: Effectiveness of elemental sublattices in lead halide perovskites.. *Journal of Chemical Physics*, **2022**, 156, 054110	3.9	3
452	Charge carrier nonadiabatic dynamics in non-metal doped graphitic carbon nitride.. *Journal of Chemical Physics*, **2022**, 156, 094702	3.9	4
451	Suppressing Oxygen-Induced Deterioration of Metal Halide Perovskites by Alkaline Earth Metal Doping: A Quantum Dynamics Study.. *Journal of the American Chemical Society*, **2022**, 144, 5543-5551	16.4	8
450	How Hole Injection Accelerates Both Ion Migration and Nonradiative Recombination in Metal Halide Perovskites.. *Journal of the American Chemical Society*, **2022**,	16.4	14
449	CO Adsorbate Promotes Polaron Photoactivity on the Reduced Rutile TiO(110) Surface.. *Jacs Au*, **2022**, 2, 234-245		6
448	Ag-Bi Charge Redistribution Creates Deep Traps in Defective CsAgBiBr: Machine Learning Analysis of Density Functional Theory.. *Journal of Physical Chemistry Letters*, **2022**, 3645-3651	6.4	3
447	Influence of intrinsic defects on the structure and dynamics of the mixed PbSn perovskite: first-principles DFT and NAMD simulations. *Journal of Materials Chemistry A*, **2021**, 10, 234-244	13	4
446	Nonadiabatic molecular dynamics analysis of hybrid Dion□acobson 2D leads iodide perovskites. *Applied Physics Letters*, **2021**, 119, 201102	3.4	3
445	Modeling Non-adiabatic Dynamics in Nanoscale and Condensed Matter Systems. *Accounts of Chemical Research*, **2021**, 54, 4239-4249	24.3	18
444	Excited-State Dynamics in Metal Halide Perovskites: A Theoretical Perspective **2021**, 1-54		
443	Identifying and Passivating Killer Defects in Pb-Free Double CsAgBiBr Perovskite. *Journal of Physical Chemistry Letters*, **2021**, 12, 10581-10588	6.4	3
442	Generating Shear Flows without Moving Parts by Thermo-osmosis in Heterogeneous Nanochannels. *Journal of Physical Chemistry Letters*, **2021**, 12, 10099-10105	6.4	2
441	Point Defects in Two-Dimensional □Phosphorus Carbide. *Journal of Physical Chemistry Letters*, **2021**, 12, 620-626	6.4	14
440	Concentric Approximation for Fast and Accurate Numerical Evaluation of Nonadiabatic Coupling with Projector Augmented-Wave Pseudopotentials. *Journal of Physical Chemistry Letters*, **2021**, 12, 3082-3089	6.4	19
439	Why Hybrid Tin-Based Perovskites Simultaneously Improve the Structural Stability and Charge Carriers' Lifetime: Ab Initio Quantum Dynamics. *ACS Applied Materials & Interfaces*, **2021**, 13, 16567-16575	9.5	5

438	Common Defects Accelerate Charge Separation and Reduce Recombination in CNT/Molecule Composites: Atomistic Quantum Dynamics. *Journal of the American Chemical Society*, **2021**, 143, 6649-6656	16.4	15
437	Water Splitting with a Single-Atom Cu/TiO Photocatalyst: Atomistic Origin of High Efficiency and Proposed Enhancement by Spin Selection. *Jacs Au*, **2021**, 1, 550-559		22
436	Strong Modulation of Band Gap, Carrier Mobility and Lifetime in Two-Dimensional Black Phosphorene through Acoustic Phonon Excitation. *Journal of Physical Chemistry Letters*, **2021**, 12, 3960-3967	6.4	9
435	Band alignment and defects influence the electron–phonon heat transport mechanisms across metal interfaces. *Applied Physics Letters*, **2021**, 118, 163503	3.4	3
434	Interpolating Nonadiabatic Molecular Dynamics Hamiltonian with Artificial Neural Networks. *Journal of Physical Chemistry Letters*, **2021**, 12, 6070-6077	6.4	15
433	Elimination of Charge Recombination Centers in Metal Halide Perovskites by Strain. *Journal of the American Chemical Society*, **2021**, 143, 9982-9990	16.4	21
432	Long-lived modulation of plasmonic absorption by ballistic thermal injection. *Nature Nanotechnology*, **2021**, 16, 47-51	28.7	20
431	Bidentate Lewis bases are preferred for passivation of MAPbI3 surfaces: A time-domain ab initio analysis. *Nano Energy*, **2021**, 79, 105491	17.1	15
430	Modeling Auger Processes with Nonadiabatic Molecular Dynamics. *Nano Letters*, **2021**, 21, 756-761	11.5	18
429	Weak Distance Dependence of Hot-Electron-Transfer Rates at the Interface between Monolayer MoS and Gold. *ACS Nano*, **2021**, 15, 819-828	16.7	9
428	Ab initio nonadiabatic molecular dynamics of charge carriers in metal halide perovskites. *Nanoscale*, **2021**, 13, 10239-10265	7.7	33
427	Tuning charge transfer and recombination in exTTF/CNT nanohybrids by choice of chalcogen: A time-domain density functional analysis. *Journal of Applied Physics*, **2021**, 129, 025501	2.5	3
426	Atomistic Mechanism of Passivation of Halide Vacancies in Lead Halide Perovskites by Alkali Ions. *Chemistry of Materials*, **2021**, 33, 1285-1292	9.6	14
425	Phonon-Mediated Interlayer Charge Separation and Recombination in a MoSe/WSe Heterostructure. *Nano Letters*, **2021**, 21, 2165-2173	11.5	22
424	Chemically Switchable n-Type and p-Type Conduction in Bismuth Selenide Nanoribbons for Thermoelectric Energy Harvesting. *ACS Nano*, **2021**, 15, 2791-2799	16.7	8
423	Dynamics of Photoexcited Small Polarons in Transition-Metal Oxides. *Journal of Physical Chemistry Letters*, **2021**, 12, 2191-2198	6.4	18
422	First-Principles Prediction of Two-Dimensional BCP and BCP: Structural Stability, Fundamental Properties, and Renewable Energy Applications. *Journal of Physical Chemistry Letters*, **2021**, 12, 3436-3442	6.4	10
421	Mixed Metals Slow Down Nonradiative Recombination in Saddle-Shaped Porphyrin Nanorings: A Time-Domain Atomistic Simulation. *Journal of Physical Chemistry C*, **2021**, 125, 16620-16628	3.8	2

420	Discovery of a Wurtzite-like CuFeSnSe Semiconductor Nanocrystal Polymorph and Implications for Related CuFeSe Materials. *ACS Nano*, **2021**,	16.7	4
419	Common Defects Accelerate Charge Carrier Recombination in CsSnI without Creating Mid-Gap States. *Journal of Physical Chemistry Letters*, **2021**, 12, 8699-8705	6.4	16
418	Facile Removal of Bulk Oxygen Vacancy Defects in Metal Oxides Driven by Hydrogen-Dopant Evaporation. *Journal of Physical Chemistry Letters*, **2021**, 12, 9579-9583	6.4	
417	Analytic Model of Nonequilibrium Charge Transport in Disordered Organic Semiconductors with Combined Energy and Off-Diagonal Disorder. *Journal of Physical Chemistry C*, **2021**, 125, 20230-20240	3.8	
416	Dependence between Structural and Electronic Properties of CsPbI: Unsupervised Machine Learning of Nonadiabatic Molecular Dynamics. *Journal of Physical Chemistry Letters*, **2021**, 12, 8672-8678	6.4	11
415	Excited-State Properties of Defected Halide Perovskite Quantum Dots: Insights from Computation. *Journal of Physical Chemistry Letters*, **2021**, 12, 1005-1011	6.4	6
414	Weak Anharmonicity Rationalizes the Temperature-Driven Acceleration of Nonradiative Dynamics in CuZnSnS Photoabsorbers.. *ACS Applied Materials & Interfaces*, **2021**, 13, 61365-61373	9.5	3
413	Significance of the Chemical Environment of an Element in Nonadiabatic Molecular Dynamics: Feature Selection and Dimensionality Reduction with Machine Learning.. *Journal of Physical Chemistry Letters*, **2021**, 12, 12026-12032	6.4	5
412	Influence of tungsten doping on nonradiative electron-hole recombination in monolayer MoSe with Se vacancies. *Journal of Chemical Physics*, **2020**, 153, 154701	3.9	3
411	Thermal smearing in DFT calculations: How small is really small? A case of La and Lu atoms adsorbed on graphene. *Materials Today Communications*, **2020**, 25, 101595	2.5	9
410	Combining Lindblad Master Equation and Surface Hopping to Evolve Distributions of Quantum Particles. *Journal of Physical Chemistry B*, **2020**, 124, 4326-4337	3.4	5
409	Structural Deformation Controls Charge Losses in MAPbI3: Unsupervised Machine Learning of Nonadiabatic Molecular Dynamics. *ACS Energy Letters*, **2020**, 5, 1930-1938	20.1	32
408	MAI Termination Favors Efficient Hole Extraction and Slow Charge Recombination at the MAPbI/CuSCN Heterojunction. *Journal of Physical Chemistry Letters*, **2020**, 11, 4481-4489	6.4	13
407	Anti-correlation between Band gap and Carrier Lifetime in Lead Halide Perovskites under Compression Rationalized by Ab Initio Quantum Dynamics. *Chemistry of Materials*, **2020**, 32, 4707-4715	9.6	20
406	Atomic fluctuations in electronic materials revealed by dephasing. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 11940-11946	11.5	16
405	Iodine and Sulfur Vacancy Cooperation Promotes Ultrafast Charge Extraction at MAPbI3/MoS2 Interface. *ACS Energy Letters*, **2020**, 5, 1346-1354	20.1	29
404	Sharp-tip enhanced catalytic CO oxidation by atomically dispersed Pt1/Pt2 on a raised graphene oxide platform. *Journal of Materials Chemistry A*, **2020**, 8, 12485-12494	13	6
403	Low-frequency lattice phonons in halide perovskites explain high defect tolerance toward electron-hole recombination. *Science Advances*, **2020**, 6, eaaw7453	14.3	99

402	Tunable Hydrogen Doping of Metal Oxide Semiconductors with Acid-Metal Treatment at Ambient Conditions. *Journal of the American Chemical Society*, **2020**, 142, 4136-4140	16.4	25
401	Pb dimerization greatly accelerates charge losses in MAPbI: Time-domain ab initio analysis. *Journal of Chemical Physics*, **2020**, 152, 064707	3.9	7
400	Improved description of hematite surfaces by the SCAN functional. *Journal of Chemical Physics*, **2020**, 152, 024706	3.9	8
399	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
398	Soft Lattice and Defect Covalency Rationalize Tolerance of CsPbI Perovskite Solar Cells to Native Defects. *Angewandte Chemie - International Edition*, **2020**, 59, 6435-6441	16.4	72
397	CO Photoreduction on Metal Oxide Surface Is Driven by Transient Capture of Hot Electrons: Quantum Dynamics Simulation. *Journal of the American Chemical Society*, **2020**, 142, 3214-3221	16.4	29
396	Control of Charge Carrier Dynamics in Plasmonic Au Films by TiO Substrate Stoichiometry. *Journal of Physical Chemistry Letters*, **2020**, 11, 1419-1427	6.4	15
395	Soft Lattice and Defect Covalency Rationalize Tolerance of CsPbI3 Perovskite Solar Cells to Native Defects. *Angewandte Chemie*, **2020**, 132, 6497-6503	3.6	6
394	Electron–phonon coupling and related transport properties of metals and intermetallic alloys from first principles. *Materials Today Physics*, **2020**, 12, 100175	8	12
393	Extending Carrier Lifetimes in Lead Halide Perovskites with Alkali Metals by Passivating and Eliminating Halide Interstitial Defects. *Angewandte Chemie - International Edition*, **2020**, 59, 4684-4690	16.4	47
392	Extending Carrier Lifetimes in Lead Halide Perovskites with Alkali Metals by Passivating and Eliminating Halide Interstitial Defects. *Angewandte Chemie*, **2020**, 132, 4714-4720	3.6	5
391	Edge Influence on Charge Carrier Localization and Lifetime in CHNHPbBr Perovskite: Quantum Dynamics Simulation. *Journal of Physical Chemistry Letters*, **2020**, 11, 9100-9109	6.4	20
390	Protecting hot carriers by tuning hybrid perovskite structures with alkali cations. *Science Advances*, **2020**, 6,	14.3	20
389	Net Unidirectional Fluid Transport in Locally Heated Nanochannel by Thermo-osmosis. *Nano Letters* , **2020**, 20, 8965-8971	11.5	11
388	Accurate Computation of Nonadiabatic Coupling with Projector Augmented-Wave Pseudopotentials. *Journal of Physical Chemistry Letters*, **2020**, 11, 10073-10080	6.4	32
387	Atomic Model for Alkali Metal Passivation of Point Defects at Perovskite Grain Boundaries. *ACS Energy Letters*, **2020**, 5, 3813-3820	20.1	26
386	Quantum dynamics origin of high photocatalytic activity of mixed-phase anatase/rutile TiO. *Journal of Chemical Physics*, **2020**, 153, 044706	3.9	18
385	Photoinduced Dynamics of Charge Carriers in Metal Halide Perovskites from an Atomistic Perspective. *Journal of Physical Chemistry Letters*, **2020**, 11, 7066-7082	6.4	28

384	Why Oxygen Increases Carrier Lifetimes but Accelerates Degradation of CHNHPbI under Light Irradiation: Time-Domain Ab Initio Analysis. *Journal of the American Chemical Society*, **2020**, 142, 14664-14673	16.4	33
383	Ab initio quantum dynamics of charge carriers in graphitic carbon nitride nanosheets. *Journal of Chemical Physics*, **2020**, 153, 054701	3.9	13
382	Long-Lived Hot Electron in a Metallic Particle for Plasmonics and Catalysis: Nonadiabatic Molecular Dynamics with Machine Learning. *ACS Nano*, **2020**, 14, 10608-10615	16.7	23
381	Electron–Phonon Relaxation at Au/Ti Interfaces Is Robust to Alloying: Ab Initio Nonadiabatic Molecular Dynamics. *Journal of Physical Chemistry C*, **2019**, 123, 22842-22850	3.8	4
380	Exciton Dissociation and Suppressed Charge Recombination at 2D Perovskite Edges: Key Roles of Unsaturated Halide Bonds and Thermal Disorder. *Journal of the American Chemical Society*, **2019**, 141, 15557-15566	16.4	66
379	Core-dependent properties of copper nanoclusters: valence-pure nanoclusters as NIR TADF emitters and mixed-valence ones as semiconductors. *Chemical Science*, **2019**, 10, 10122-10128	9.4	13
378	Suppression of Electron-Hole Recombination by Intrinsic Defects in 2D Monoelemental Material. *Journal of Physical Chemistry Letters*, **2019**, 10, 6151-6158	6.4	39
377	Size-Programmed Synthesis of PbSe Quantum Dots via Secondary Phosphine Chalcogenides. *Chemistry of Materials*, **2019**, 31, 8301-8307	9.6	4
376	Numerical tests of coherence-corrected surface hopping methods using a donor-bridge-acceptor model system. *Journal of Chemical Physics*, **2019**, 150, 194104	3.9	12
375	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
374	Ehrenfest and classical path dynamics with decoherence and detailed balance. *Journal of Chemical Physics*, **2019**, 150, 204124	3.9	27
373	Strong Influence of Oxygen Vacancy Location on Charge Carrier Losses in Reduced TiO Nanoparticles. *Journal of Physical Chemistry Letters*, **2019**, 10, 2676-2683	6.4	21
372	Thin Ti adhesion layer breaks bottleneck to hot hole relaxation in Au films. *Journal of Chemical Physics*, **2019**, 150, 184701	3.9	9
371	Coexistence of Different Charge-Transfer Mechanisms in the Hot-Carrier Dynamics of Hybrid Plasmonic Nanomaterials. *Nano Letters*, **2019**, 19, 3187-3193	11.5	23
370	First-principles determination of the ultrahigh electrical and thermal conductivity in free-electron metals via pressure tuning the electron-phonon coupling factor. *Physical Review B*, **2019**, 99,	3.3	11
369	Superoxide/Peroxide Chemistry Extends Charge Carriers' Lifetime but Undermines Chemical Stability of CHNHPbI Exposed to Oxygen: Time-Domain ab Initio Analysis. *Journal of the American Chemical Society*, **2019**, 141, 5798-5807	16.4	80
368	Symmetry Breaking at MAPbI Perovskite Grain Boundaries Suppresses Charge Recombination: Time-Domain ab Initio Analysis. *Journal of Physical Chemistry Letters*, **2019**, 10, 1617-1623	6.4	53
367	Catalytic Chemistry Predicted by a Charge Polarization Descriptor: Synergistic O Activation and CO Oxidation by Au-Cu Bimetallic Clusters on TiO(101). *ACS Applied Materials & Interfaces*, **2019**, 11, 9629-9640	9.5	18

366	Lattice Expansion in Hybrid Perovskites: Effect on Optoelectronic Properties and Charge Carrier Dynamics. *Journal of Physical Chemistry Letters*, **2019**, 10, 5000-5007	6.4	38
365	Phonon-Suppressed Auger Scattering of Charge Carriers in Defective Two-Dimensional Transition Metal Dichalcogenides. *Nano Letters*, **2019**, 19, 6078-6086	11.5	27
364	The Periodic Table. *Journal of Physical Chemistry A*, **2019**, 123, 5837-5848	2.8	1
363	Triplet Excitons in Small Helium Clusters. *Journal of Physical Chemistry A*, **2019**, 123, 6113-6122	2.8	
362	The JPC Periodic Table. *Journal of Physical Chemistry C*, **2019**, 123, 17063-17074	3.8	1
361	The JPC Periodic Table. *Journal of Physical Chemistry Letters*, **2019**, 10, 4051-4062	6.4	1
360	Anharmonicity Extends Carrier Lifetimes in Lead Halide Perovskites at Elevated Temperatures. *Journal of Physical Chemistry Letters*, **2019**, 10, 6219-6226	6.4	41
359	Electron-Phonon Scattering Is Much Weaker in Carbon Nanotubes than in Graphene Nanoribbons. *Journal of Physical Chemistry Letters*, **2019**, 10, 7179-7187	6.4	14
358	Enhanced Activity of CN-Supported Single Co Atom Catalyst by Single Atom Promoter. *Journal of Physical Chemistry Letters*, **2019**, 10, 7009-7014	6.4	17
357	Mono-Elemental Properties of 2D Black Phosphorus Ensure Extended Charge Carrier Lifetimes under Oxidation: Time-Domain Ab Initio Analysis. *Journal of Physical Chemistry Letters*, **2019**, 10, 1083-1091	6.4	55
356	Dependence of electron transfer dynamics on the number of graphene layers in stacked 2D materials: insights from ab initio nonadiabatic molecular dynamics. *Physical Chemistry Chemical Physics*, **2019**, 21, 23198-23208	3.6	6
355	Strain Controls Charge Carrier Lifetimes in Monolayer WSe: Ab Initio Time Domain Analysis. *Journal of Physical Chemistry Letters*, **2019**, 10, 7732-7739	6.4	22
354	Why Silicon Doping Accelerates Electron Polaron Diffusion in Hematite. *Journal of the American Chemical Society*, **2019**, 141, 20222-20233	16.4	27
353	JPCL: A Dynamic Journal with a Global Reach. *Journal of Physical Chemistry Letters*, **2019**, 10, 113-114	6.4	
352	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
351	Molecular Photophysics under Shock Compression: Ab Initio Nonadiabatic Molecular Dynamics of Rhodamine Dye. *Journal of Physical Chemistry C*, **2018**, 122, 13600-13607	3.8	2
350	DFT study of the infrared and Raman spectra of photochromic Fulgide; 3-Dicyclopropylmethylene-4-E-[1-(2,5-dimethyl-3-furyl)ethylidene]-5-(4-nitrophenylcyanomethylenetetrahydrofuran-2-or *Structural Chemistry*, **2018**, 29, 1085-1094	1.8	1
349	Size and Shape Effects on Charge Recombination Dynamics of TiO2 Nanoclusters. *Journal of Physical Chemistry C*, **2018**, 122, 5201-5208	3.8	24

348	Delocalized Impurity Phonon Induced Electron-Hole Recombination in Doped Semiconductors. *Nano Letters*, **2018**, 18, 1592-1599	11.5	63
347	Plasmon-Mediated Electron Injection from Au Nanorods into MoS2: Traditional versus Photoexcitation Mechanism. *CheM*, **2018**, 4, 1112-1127	16.2	56
346	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
345	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
344	Recent theoretical progress in the development of perovskite photovoltaic materials. *Journal of Energy Chemistry*, **2018**, 27, 637-649	12	32
343	Increased Lattice Stiffness Suppresses Nonradiative Charge Recombination in MAPbI3 Doped with Larger Cations: Time-Domain Ab Initio Analysis. *ACS Energy Letters*, **2018**, 3, 2070-2076	20.1	53
342	Long Carrier Lifetimes in PbI2-Rich Perovskites Rationalized by Ab Initio Nonadiabatic Molecular Dynamics. *ACS Energy Letters*, **2018**, 3, 1868-1874	20.1	41
341	Spin□Orbit Interactions Greatly Accelerate Nonradiative Dynamics in Lead Halide Perovskites. *ACS Energy Letters*, **2018**, 3, 2159-2166	20.1	82
340	Superatom Molecular Orbital as an Interfacial Charge Separation State. *Journal of Physical Chemistry Letters*, **2018**, 9, 3485-3490	6.4	24
339	Real-Time Atomistic Dynamics of Energy Flow in an STM Setup: Revealing the Mechanism of Current-Induced Molecular Emission. *Journal of Physical Chemistry Letters*, **2018**, 9, 3591-3597	6.4	10
338	Photoexcited Nonadiabatic Dynamics of Solvated Push-Pull □Conjugated Oligomers with the NEXMD Software. *Journal of Chemical Theory and Computation*, **2018**, 14, 3955-3966	6.4	30
337	Ultrafast, asymmetric charge transfer and slow charge recombination in porphyrin/CNT composites demonstrated by time-domain atomistic simulation. *Nanoscale*, **2018**, 10, 12683-12694	7.7	17
336	Theoretical Investigation of Relaxation Dynamics in Au38(SH)24 Thiolate-Protected Gold Nanoclusters. *Journal of Physical Chemistry C*, **2018**, 122, 16380-16388	3.8	19
335	Effect of Aspect Ratio on Multiparticle Auger Recombination in Single-Walled Carbon Nanotubes: Time Domain Atomistic Simulation. *Nano Letters*, **2018**, 18, 58-63	11.5	27
334	Hot Electron Thermoreflectance Coefficient of Gold during Electron□Phonon Nonequilibrium. *ACS Photonics*, **2018**, 5, 4880-4887	6.3	13
333	Conversion of He(2 S) to He(a□) in Liquid Helium. *Journal of Physical Chemistry Letters*, **2018**, 9, 6017-6023	6.4	4
332	Time-Domain ab Initio Analysis Rationalizes the Unusual Temperature Dependence of Charge Carrier Relaxation in Lead Halide Perovskite. *ACS Energy Letters*, **2018**, 3, 2713-2720	20.1	47
331	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

330	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	3.8	12
329	Phonon-coupled ultrafast interlayer charge oscillation at van der Waals heterostructure interfaces. *Physical Review B*, **2018**, 97,	3.3	51
328	Why Chemical Vapor Deposition Grown MoS Samples Outperform Physical Vapor Deposition Samples: Time-Domain ab Initio Analysis. *Nano Letters*, **2018**, 18, 4008-4014	11.5	56
327	C2N-supported single metal ion catalysts for HCOOH dehydrogenation. *Journal of Materials Chemistry A*, **2018**, 6, 11105-11112	13	28
326	Hot-Hole Cooling Controls the Initial Ultrafast Relaxation in Methylammonium Lead Iodide Perovskite. *Scientific Reports*, **2018**, 8, 8115	4.9	26
325	Influence of Encapsulated Water on Luminescence Energy, Line Width, and Lifetime of Carbon Nanotubes: Time Domain Ab Initio Analysis. *Journal of Physical Chemistry Letters*, **2018**, 9, 4006-4013	6.4	18
324	Ferroelectric Alignment of Organic Cations Inhibits Nonradiative Electron-Hole Recombination in Hybrid Perovskites: Ab Initio Nonadiabatic Molecular Dynamics. *Journal of Physical Chemistry Letters*, **2017**, 8, 812-818	6.4	48
323	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
322	Microwave reduction of graphene oxide rationalized by reactive molecular dynamics. *Nanoscale*, **2017**, 9, 4024-4033	7.7	20
321	Atomistic Analysis of Room Temperature Quantum Coherence in Two-Dimensional CdSe Nanostructures. *Nano Letters*, **2017**, 17, 2389-2396	11.5	24
320	Two-Dimensional Linear Dichroism Spectroscopy for Identifying Protein Orientation and Secondary Structure Composition. *Journal of Physical Chemistry Letters*, **2017**, 8, 1031-1037	6.4	5
319	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
318	Cooperative enhancement of the nonlinear optical response in conjugated energetic materials: A TD-DFT study. *Journal of Chemical Physics*, **2017**, 146, 114308	3.9	8
317	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
316	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
315	Weak Donor-Acceptor Interaction and Interface Polarization Define Photoexcitation Dynamics in the MoS/TiO Composite: Time-Domain Ab Initio Simulation. *Nano Letters*, **2017**, 17, 4038-4046	11.5	41
314	Quantum Dynamics of Photogenerated Charge Carriers in Hybrid Perovskites: Dopants, Grain Boundaries, Electric Order, and Other Realistic Aspects. *ACS Energy Letters*, **2017**, 2, 1588-1597	20.1	25
313	Imidazolium Ionic Liquid Mediates Black Phosphorus Exfoliation while Preventing Phosphorene Decomposition. *ACS Nano*, **2017**, 11, 6459-6466	16.7	31

312	Nonadiabatic charge dynamics in novel solar cell materials. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2017**, 7, e1305	7.9	53
311	Analytic Modeling of Field Dependence of Charge Mobility and Applicability of the Concept of the Effective Transport Level to an Organic Dipole Glass. *Journal of Physical Chemistry C*, **2017**, 121, 7776-7781	3.8	7
310	Time-Domain ab Initio Modeling of Electron-Phonon Relaxation in High-Temperature Cuprate Superconductors. *Journal of Physical Chemistry Letters*, **2017**, 8, 193-198	6.4	19
309	The JPCL New Year's Editorial. *Journal of Physical Chemistry Letters*, **2017**, 8, 41	6.4	
308	Exfoliation of Graphene in Ionic Liquids: Pyridinium versus Pyrrolidinium. *Journal of Physical Chemistry C*, **2017**, 121, 911-917	3.8	23
307	Perspective Collections in the Limelight. *Journal of Physical Chemistry Letters*, **2017**, 8, 5239-5239	6.4	
306	In the Limelight. *Journal of Physical Chemistry Letters*, **2017**, 8, 3925-3925	6.4	
305	Phonon-Assisted Ultrafast Charge Transfer at van der Waals Heterostructure Interface. *Nano Letters*, **2017**, 17, 6435-6442	11.5	120
304	Temperature Dependence of Electron□Phonon Interactions in Gold Films Rationalized by Time-Domain Ab Initio Analysis. *Journal of Physical Chemistry C*, **2017**, 121, 17488-17497	3.8	15
303	Role of Methylammonium Orientation in Ion Diffusion and Current□Voltage Hysteresis in the CH3NH3PbI3 Perovskite. *ACS Energy Letters*, **2017**, 2, 1997-2004	20.1	55
302	Optoelectronic Properties of Semiconductor Quantum Dot Solids for Photovoltaic Applications. *Journal of Physical Chemistry Letters*, **2017**, 8, 4129-4139	6.4	49
301	In the Limelight. *Journal of Physical Chemistry Letters*, **2017**, 8, 3718-3719	6.4	
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