Alexander J White

List of Publications by Year
in descending order

31 papers	847 citations	471509 17 h-index	477307 29 g-index
32 all docs	32 docs citations	32 times ranked	759 citing authors

#	Article	IF	Citations
1	Non-adiabatic Excited-State Molecular Dynamics: Theory and Applications for Modeling Photophysics in Extended Molecular Materials. Chemical Reviews, 2020, 120, 2215-2287.	47.7	231
2	NEXMD Software Package for Nonadiabatic Excited State Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2020, 16, 5771-5783.	5.3	56
3	Collective Plasmon-Molecule Excitations in Nanojunctions: Quantum Consideration. Journal of Physical Chemistry Letters, 2012, 3, 2738-2743.	4.6	51
4	AbÂInitio Studies on the Stopping Power of Warm Dense Matter with Time-Dependent Orbital-Free Density Functional Theory. Physical Review Letters, 2018, 121, 145001.	7.8	44
5	Review of the first charged-particle transport coefficient comparison workshop. High Energy Density Physics, 2020, 37, 100905.	1.5	42
6	Photoexcited Nonadiabatic Dynamics of Solvated Pushâ€“Pull Ï€-Conjugated Oligomers with the NEXMD Software. Journal of Chemical Theory and Computation, 2018, 14, 3955-3966.	5.3	39
7	Inelastic transport: a pseudoparticle approach. Physical Chemistry Chemical Physics, 2012, 14, 13809.	2.8	37
8	Raman Scattering in Molecular Junctions: A Pseudoparticle Formulation. Nano Letters, 2014, 14, 699-703.	9.1	30
9	Time-dependent orbital-free density functional theory for electronic stopping power: Comparison to the Mermin-Kohn-Sham theory at high temperatures. Physical Review B, 2018, 98, .	3.2	27
10	Fast and Universal Kohn-Sham Density Functional Theory Algorithm for Warm Dense Matter to Hot Dense Plasma. Physical Review Letters, 2020, 125, 055002.	7.8	27
11	Coherence in charge and energy transfer in molecular junctions. Physical Review B, 2013, 88, .	3.2	26
12	Correlation and transport properties for mixtures at constant pressure and temperature. Physical Review E, 2017, 95, 063202.	2.1	24
13	Nonequilibrium Atomic Limit for Transport and Optical Response of Molecular Junctions. Journal of Physical Chemistry C, 2014, 118, 11159-11173.	3.1	21
14	Molecular nanoplasmonics: Self-consistent electrodynamics in current-carrying junctions. Physical Review B, 2012, 86, .	3.2	20
15	Nonadiabatic Excited-State Molecular Dynamics Methodologies: Comparison and Convergence. Journal of Physical Chemistry Letters, 2021, 12, 2970-2982.	4.6	20
16	Coupled wave-packets for non-adiabatic molecular dynamics: a generalization of Gaussian wave-packet dynamics to multiple potential energy surfaces. Chemical Science, 2016, 7, 4905-4911.	7.4	18
17	Semiclassical Monte Carlo: A first principles approach to non-adiabatic molecular dynamics. Journal of Chemical Physics, 2014, 141, 184101.	3.0	17
18	An Ab Initio Multiple Cloning Method for Non-Adiabatic Excited-State Molecular Dynamics in NWChem. Journal of Chemical Theory and Computation, 2021, 17, 3629-3643.	5.3	15

#	Article	IF	Citations
19	Quantum transport with two interacting conduction channels. Journal of Chemical Physics, 2013, 138, 174111.	3.0	14
20	Non-adiabatic molecular dynamics by accelerated semiclassical Monte Carlo. Journal of Chemical Physics, 2015, 143, 014115.	3.0	13
21	Multicomponent mutual diffusion in the warm, dense matter regime. Physical Review E, 2019, 100, 033213.	2.1	13
22	Static and dynamic properties of multi-ionic plasma mixtures. Physical Review E, 2020, 101, 033207.	2.1	13
23	Proton stopping measurements at low velocity in warm dense carbon. Nature Communications, 2022, 13, .	12.8	13
24	Improved Ehrenfest Approach to Model Correlated Electronâ€“Nuclear Dynamics. Journal of Physical Chemistry Letters, 2019, 10, 433-440.	4.6	10
25	Effects of Electromagnetic Coupling on Conductance Switching of a Gated Tunnel Junction. Journal of Physical Chemistry Letters, 2014, 5, 3545-3550.	4.6	6
26	Mixed Stochastic-Deterministic Time-Dependent Density Functional Theory: Application to Stopping Power of Warm Dense Carbon. Journal of Physics Condensed Matter, 2022, , .	1.8	6
27	Enhancement of nuclear reaction rates in asymmetric binary ionic mixtures. Contributions To Plasma Physics, 2017, 57, 512-517.	1.1	5
28	Enhancement factor of nuclear reactions in partially ionized plasmas and asymmetric mixtures. Contributions To Plasma Physics, 2019, 59, e201800155.	1.1	3
29	Checking the Salpeter enhancement of nuclear reactions at intermediate coupling in asymmetric mixtures. Physics of Plasmas, 2019, 26, 012702.	1.9	3
30	Mixed quantumâ€“classical approach to model non-adiabatic electronâ€“nuclear dynamics: Detailed balance and improved surface hopping method. Journal of Chemical Physics, 2020, 153, 074116.	3.0	2
31	Non-Markovian theory of collective plasmon-molecule excitations in nanojunctions combined with classical electrodynamic simulations. , 2013, , .		1