Igor V Schweigert

List of Publications by Year
in descending order

34	999	471509 17	414414 32
papers	citations	h-index	g-index

35	35	35	1219
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Ab initiodensity functional theory: The best of both worlds?. Journal of Chemical Physics, 2005, 123, 062205.	3.0	160
2	Coherent Multidimensional Optical Probes for Electron Correlations and Exciton Dynamics: From NMR to X-rays. Accounts of Chemical Research, 2009, 42, 553-562.	15.6	90
3	Coherent Ultrafast Core-Hole Correlation Spectroscopy: X-Ray Analogues of Multidimensional NMR. Physical Review Letters, 2007, 99, 163001.	7.8	73
4	Probing valence electronic wave-packet dynamics by all x-ray stimulated Raman spectroscopy: A simulation study. Physical Review A, 2007, 76, .	2.5	67
5	Coarse-Grain Model Simulations of Nonequilibrium Dynamics in Heterogeneous Materials. Journal of Physical Chemistry Letters, 2014, 5, 2144-2149.	4.6	59
6	Ab initio correlation functionals from second-order perturbation theory. Journal of Chemical Physics, 2006, 125, 104108.	3.0	58
7	Two-dimensional optical spectroscopy of excitons in semiconductor quantum wells: Liouville-space pathway analysis. Physical Review B, 2007, 75, .	3.2	57
8	Ab initio DFT: Getting the right answer for the right reason. Computational and Theoretical Chemistry, 2006, 771, 1-8.	1.5	49
9	Fermi resonance in CO2: A combined electronic coupled-cluster and vibrational configuration-interaction prediction. Journal of Chemical Physics, 2007, 126, 124303.	3.0	47
10	Ab Initio Molecular Dynamics of High-Temperature Unimolecular Dissociation of Gas-Phase RDX and Its Dissociation Products. Journal of Physical Chemistry A, 2015, 119, 2747-2759.	2.5	47
11	Simulating multidimensional optical wave-mixing signals with finite-pulse envelopes. Physical Review A, 2008, 77, .	2.5	26
12	Double-quantum-coherence attosecond x-ray spectroscopy of spatially separated, spectrally overlapping core-electron transitions. Physical Review A, 2008, 78, .	2.5	26
13	Hydrolysis of Dimethyl Methylphosphonate by the Cyclic Tetramer of Zirconium Hydroxide. Journal of Physical Chemistry A, 2017, 121, 7690-7696.	2.5	26
14	Kinetics of Dimethyl Methylphosphonate Adsorption and Decomposition on Zirconium Hydroxide Using Variable Temperature In Situ Attenuated Total Reflection Infrared Spectroscopy. ACS Applied Materials & Interfaces, 2020, 12, 14662-14671.	8.0	23
15	Evaluation of reaction kinetics models for meso-scale simulations of hotspot initiation and growth in HMX. Combustion and Flame, 2020, 219, 225-241.	5.2	22
16	Probing Multiple Coreâ^'Hole Interactions in the Nitrogen K-Edge of DNA Base Pairs by Multidimensional Attosecond X-ray Spectroscopy. A Simulation Study. Journal of Physical Chemistry A, 2008, 112, 11449-11461.	2.5	21
17	Dissipative particle dynamics with reactions: Application to RDX decomposition. Journal of Chemical Physics, 2019, 151, 114112.	3.0	20
18	Effect of the nonlocal exchange on the performance of the orbital-dependent correlation functionals from second-order perturbation theory. Journal of Chemical Physics, 2008, 129, 124109.	3.0	17

#	Article	IF	Citations
19	Probing interactions between core-electron transitions by ultrafast two-dimensional x-ray coherent correlation spectroscopy. Journal of Chemical Physics, 2008, 128, 184307.	3.0	15
20	Electronic structure and molecular dynamics of breaking the ROâ€“NO2 bond. Journal of Chemical Physics, 2009, 130, 244110.	3.0	14
21	Thermodynamic and kinetic stabilities of CO2 oligomers. Journal of Chemical Physics, 2013, 138, 134304.	3.0	11
22	Quantum mechanical simulations of condensed-phase decomposition dynamics in molten RDX. Journal of Physics: Conference Series, 2014, 500, 052039.	0.4	11
23	Modeling Electronic Trap States at Interfaces between Anatase Nanoparticles. Journal of Physical Chemistry C, 2017, 121, 14254-14260.	3.1	10
24	Vibrational Signatures of Sarin Adsorption on Anatase Surfaces. Surface Science, 2021, 705, 121765.	1.9	9
25	Interconnection between functional derivative and effective operator approaches toab initiodensity functional theory. Molecular Physics, 2005, 103, 2299-2307.	1.7	8
26	Battling Chemical Weapons with Zirconium Hydroxide Nanoparticle Sorbent: Impact of Environmental Contaminants on Sarin Sequestration and Decomposition. Langmuir, 2021, 37, 6923-6934.	3.5	8
27	Self-consistent, constrained linear-combination-of-atomic-potentials approach to quantum mechanics. Journal of Chemical Physics, 2011, 134, 044122.	3.0	6
28	Adsorption of organophosphate nerve agent VX on the (101) surface of anatase titanium dioxide. Surface Science, 2022, 716, 121957.	1.9	6
29	Molecular dynamics simulations of rapidly heated RDX. AIP Conference Proceedings, 2018, , .	0.4	4
30	Bimolecular Reactions between Dimethylnitramine and Its Radical Decomposition Products. Journal of Physical Chemistry A, 2017, 121, 1544-1552.	2.5	3
31	Mechanisms of condensed-phase dissociation of nitramines: A density-functional study. , 2012, , .		2
32	Shock simulations of a single-site coarse-grain RDX model using the dissipative particle dynamics method with reactivity. AIP Conference Proceedings, 2017, , .	0.4	2
33	Modeling solidâ€“solid phase transitions in PETN using density functional theory. AIP Conference Proceedings, 2018, , .	0.4	2
34	Shattering dissociation in high-energy molecular collisions between nitrate esters. Journal of Chemical Physics, 2011, 135, 114306.	3.0	0