Tillmann Klamroth

List of Publications by Year
in descending order

27	823	623734 14	526287 27
papers	citations	h-index	g-index

28	28	28	678
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Many-electron dynamics in laser-driven molecules: wavefunction theory vs. density functional theory. Physical Chemistry Chemical Physics, 2021, 23, 13544-13560.	2.8	19
2	Nonlocal STM Manipulation of Chlorobenzene on Si(111)-7 Ã— 7: Potentials, Kinetics, and First-Principles Molecular Dynamics Calculations for Open Systems. Journal of Physical Chemistry C, 2021, 125, 12175-12184.	3.1	1
3	Gaussian-Type Orbital Calculations for High Harmonic Generation in Vibrating Molecules: Benchmarks for H₂⁺. Journal of Chemical Theory and Computation, 2021, 17, 7353-7365.	5.3	6
4	<scp>PSIXAS</scp>: A Psi4 plugin for efficient simulations of Xâ€ray absorption spectra based on the transitionâ€potential and <scp>Î”â€Kohnâ€“Sham</scp> method. Journal of Computational Chemistry, 2020, 41, 1781-1789.	3.3	21
5	Molecular attochemistry: Correlated electron dynamics driven by light. Advances in Quantum Chemistry, 2020, 81, 15-50.	0.8	15
6	Discriminating organic isomers by high harmonic generation: A time-dependent configuration interaction singles study. Journal of Chemical Physics, 2019, 150, 234114.	3.0	21
7	Local resonances in STM manipulation of chlorobenzene on Si(111)-7Ã—7: performance of different cluster models and density functionals. Molecular Physics, 2018, 116, 1687-1696.	1.7	3
8	Quantum dynamics, isotope effects, and power spectra of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msup><mml:mrow /><mml:mo>+</mml:mo></mml:msup></mml:mrow></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mrow><mml:mi>HD</mml:mi></mml:mrow><mml:mo>+</mml:mo></mml:msup></mml:math> excited to the continuum by strong one-cycle laser pulses: Three-dimensional non-. Physical Review A,	2.5	12
9	Desorption induced by low energy charge carriers on Si(111)â€7 Ã— 7: First principles molecular dynamics for benzene derivates. Journal of Computational Chemistry, 2018, 39, 2517-2525.	3.3	5
10	The quest for best suited references for configuration interaction singles calculations of core excited states. Journal of Computational Chemistry, 2017, 38, 116-126.	3.3	12
11	Controlling the high frequency response of H2 by ultra-short tailored laser pulses: A time-dependent configuration interaction study. Journal of Chemical Physics, 2016, 144, 044301.	3.0	11
12	Tetrahalidocuprates(ii) â€“ structure and EPR spectroscopy. Part 2: tetrachloridocuprates(ii). New Journal of Chemistry, 2014, 38, 1019.	2.8	31
13	Laser Control for Coupled Torsions in Chiroptical Switches: A Combined Quantum and Classical Dynamics Approach. Journal of Physical Chemistry C, 2014, 118, 1322-1331.	3.1	1
14	Quantum Chemical Cluster Models for Chemi- and Physisorption of Chlorobenzene on Si(111)-7Ã—7. Journal of Physical Chemistry A, 2014, 118, 6699-6704.	2.5	6
15	SIMULATIONS OF PUMP-PROBE EXCITATIONS OF ELECTRONIC WAVE PACKETS FOR A LARGE QUASI-RIGID MOLECULAR SYSTEM BY MEANS OF AN EXTENSION TO THE TIME-DEPENDENT CONFIGURATION INTERACTION SINGLES METHOD. Journal of Theoretical and Computational Chemistry, 2013, 12, 1350005.	1.8	4
16	Current versus temperature-induced switching of a single molecule: Open-system density matrix theory for 1,5-cyclooctadiene on Si(100). Journal of Chemical Physics, 2012, 136, 094705.	3.0	6
17	Complexation of Palladium(II) with Unsaturated Dithioethers â€“ A Systematic Development of Highly Selective Ligands for Solvent Extraction. European Journal of Inorganic Chemistry, 2012, 2012, 2341-2352.	2.0	24
18	Tetrahalidocuprates(ii)â€”structure and EPR spectroscopy. Part 1: Tetrabromidocuprates(ii). New Journal of Chemistry, 2011, 35, 2793.	2.8	23

#	Article	IF	Citations
19	Time-dependent response of dissipative electron systems. Physical Review A, 2010, 81, .	2.5	21
20	Photoisomerization Ability of Molecular Switches Adsorbed on Au(111): Comparison between Azobenzene and Stilbene Derivatives. Journal of Physical Chemistry C, 2010, 114, 1231-1239.	3.1	46
21	Laser-induced electron dynamics including photoionization: A heuristic model within time-dependent configuration interaction theory. Journal of Chemical Physics, 2009, 131, 114304.	3.0	72
22	Current versus Temperature-Induced Switching in a Single-Molecule Tunnel Junction: 1,5 Cyclooctadiene on Si(001). Nano Letters, 2009, 9, 2996-3000.	9.1	30
23	Stereoselective isomerization of an ensemble of adsorbed molecules with multiple orientations: Stochastic laser pulse optimization for selective switching between achiral and chiral atropisomers. Journal of Chemical Physics, 2008, 129, 234701.	3.0	6
24	Molecular response properties from explicitly time-dependent configuration interaction methods. Journal of Chemical Physics, 2007, 127, 034107.	3.0	98
25	On the Electronic Structure of Neutral and Ionic Azobenzenes and Their Possible Role as Surface Mounted Molecular Switches. Journal of Physical Chemistry B, 2006, 110, 16337-16345.	2.6	80
26	Time-dependent configuration-interaction calculations of laser-pulse-driven many-electron dynamics: Controlled dipole switching in lithium cyanide. Journal of Chemical Physics, 2005, 123, 074105.	3.0	163
27	Laser-driven electron transfer through metal-insulator-metal contacts: Time-dependent configuration interaction singles calculations for a jellium model. Physical Review B, 2003, 68, .	3.2	86