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	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
2	Molecular response properties from explicitly time-dependent configuration interaction methods. Journal of Chemical Physics, 2007, 127, 034107.	3.0	98
3	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
4	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
5	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
6	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
7	Tetrahalidocuprates(ii) â€“ structure and EPR spectroscopy. Part 2: tetrachloridocuprates(ii). New Journal of Chemistry, 2014, 38, 1019.	2.8	31
8	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
9	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
10	Tetrahalidocuprates(ii)â€”structure and EPR spectroscopy. Part 1: Tetrabromidocuprates(ii). New Journal of Chemistry, 2011, 35, 2793.	2.8	23
11	Time-dependent response of dissipative electron systems. Physical Review A, 2010, 81, .	2.5	21
12	Discriminating organic isomers by high harmonic generation: A time-dependent configuration interaction singles study. Journal of Chemical Physics, 2019, 150, 234114.	3.0	21
13	<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
14	Many-electron dynamics in laser-driven molecules: wavefunction theory vs. density functional theory. Physical Chemistry Chemical Physics, 2021, 23, 13544-13560.	2.8	19
15	Molecular attochemistry: Correlated electron dynamics driven by light. Advances in Quantum Chemistry, 2020, 81, 15-50.	0.8	15
16	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
17	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:m excited to the continuum by strong one-cycle laser pulses: Three-dimensional non-. Physical Review A,	2.5	12
18	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

#	Article	IF	Citations
19	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
20	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
21	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
22	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
23	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
24	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
25	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
26	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
27	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