Katharine L C Hunt

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/3660312/publications.pdf

Version: 2024-02-01

48 papers	838 citations	567144 15 h-index	477173 29 g-index
48 all docs	48 docs citations	48 times ranked	633 citing authors

#	Article	IF	Citations
1	Collision-Induced Absorption by H₂ Pairs: From Hundreds to Thousands of Kelvin. Journal of Physical Chemistry A, 2011, 115, 6805-6812.	1.1	110
2	Infrared absorption by collisional H2â€“He complexes at temperatures up to 9000 K and frequencies from 0 to 20Â000 cmâ˜'1. Journal of Chemical Physics, 2012, 136, 044319.	1.2	82
3	Path integral solutions of stochastic equations for nonlinear irreversible processes: The uniqueness of the thermodynamic Lagrangian. Journal of Chemical Physics, 1981, 75, 976-984.	1.2	71
4	Dispersion dipoles and dispersion forces: Proof of Feynmanâ€™s â€˜â€˜conjectureâ€™â€™ and generalization to interacting molecules of arbitrary symmetry. Journal of Chemical Physics, 1990, 92, 1180-1187.	1.2	65
5	Thermodynamics far from equilibrium: Reactions with multiple stationary states. Journal of Chemical Physics, 1988, 88, 2719-2729.	1.2	59
6	Thermodynamic and stochastic theory for nonequilibrium systems with multiple reactive intermediates: The concept and role of excess work. Journal of Chemical Physics, 1992, 96, 618-629.	1.2	50
7	Thermodynamic and stochastic theory for nonequilibrium systems with more than one reactive intermediate: Nonautocatalytic or equilibrating systems. Journal of Chemical Physics, 1990, 92, 2572-2581.	1.2	37
8	Longâ€range, collisionâ€induced hyperpolarizabilities of atoms or centrosymmetric linear molecules: Theory and numerical results for pairs containing H or He. Journal of Chemical Physics, 1996, 105, 10954-10968.	1.2	35
9	Thermodynamic and stochastic theory of nonequilibrium systems: Fluctuation probabilities and excess work. Journal of Chemical Physics, 1995, 102, 4548-4562.	1.2	27
10	Quantum mechanical calculation of the collision-induced absorption spectra of N2â€“N2 with anisotropic interactions. Journal of Chemical Physics, 2015, 142, 084306.	1.2	26
11	Stationary solutions of the master equation for single and multiâ€intermediate autocatalytic chemical systems. Journal of Chemical Physics, 1992, 96, 630-640.	1.2	23
12	Roto-translational Raman spectra of pairs of hydrogen molecules from first principles. Journal of Chemical Physics, 2009, 130, 164314.	1.2	23
13	Infrared atmospheric emission and absorption by simple molecular complexes, from first principles. Molecular Physics, 2010, 108, 2265-2272.	0.8	21
14	Thermodynamic and stochastic theory of nonequilibrium systems: A Lagrangian approach to fluctuations and relation to excess work. Journal of Chemical Physics, 1995, 102, 4563-4573.	1.2	19
15	Multiple steady states in coupled flow tank reactors. Journal of Chemical Physics, 1992, 96, 7019-7033.	1.2	18
16	Vibrational circular dichroism and electricâ€field shielding tensors: A new physical interpretation based on nonlocal susceptibility densities. Journal of Chemical Physics, 1991, 94, 6995-7002.	1.2	14
17	Molecular quadrupole moments of HCCH, FCCF, and ClCCCl. International Journal of Quantum Chemistry, 2003, 95, 697-705.	1.0	14
18	Ab initio investigation of titanium hydroxide isomers and their cations, TiOH0, + and HTiO0, +. Journal of Chemical Physics, 2011, 135, 144111.	1.2	11

#	Article	IF	Citations
19	Interaction-induced dipoles of hydrogen molecules colliding with helium atoms: A new ab initio dipole surface for high-temperature applications. Journal of Chemical Physics, 2012, 136, 044320.	1.2	11
20	Adiabatic and nonadiabatic contributions to the energy of a system subject to a time-dependent perturbation: Complete separation and physical interpretation. Journal of Chemical Physics, 2012, 137, 164109.	1.2	11
21	Non-adiabatic current densities, transitions, and power absorbed by a molecule in a time-dependent electromagnetic field. Journal of Chemical Physics, 2015, 143, 034102.	1.2	10
22	On Liapunov functions for singleâ€variable reacting systems displaced from equilibrium. Journal of Chemical Physics, 1989, 90, 880-887.	1.2	9
23	The energy as a functional of the charge density and the charge-density susceptibility: A simple, exact, nonlocal expression for the electronic energy of a molecule. Journal of Chemical Physics, 2002, 116, 5440-5447.	1.2	9
24	Nonlocal dielectric functions on the nanoscale: Screened forces from unscreened potentials. Journal of Chemical Physics, 2003, 119, 8250-8256.	1.2	9
25	Dependence of the multipole moments, static polarizabilities, and static hyperpolarizabilities of the hydrogen molecule on the Hâ€“H separation in the ground singlet state. Journal of Chemical Physics, 2018, 149, 234103.	1.2	9
26	Determination of Thermodynamic and Stochastic Potentials in Nonequilibrium Systems from Macroscopic Measurementsâ€. Journal of Physical Chemistry A, 2002, 106, 10951-10960.	1.1	8
27	Gauge-invariant expectation values of the energy of a molecule in an electromagnetic field. Journal of Chemical Physics, 2016, 144, 044109.	1.2	8
28	First-Principles Calculations of the Electronic and Geometrical Structures of Neutral [Sc,O,H] Molecules and the Monocations, ScOH^{0,+} and HScO^{0,+}. Journal of Physical Chemistry A, 2011, 115, 4436-4447.	1.1	7
29	Note: Computation of collision-induced absorption by dense deuteriumâ€“helium gas mixtures. Journal of Chemical Physics, 2011, 134, 076101.	1.2	7
30	Path integral solutions for Fokkerâ€“Planck conditional propagators in nonequilibrium systems: Catastrophic divergences of the Onsagerâ€“Machlupâ€“Laplace approximation. Journal of Chemical Physics, 1983, 79, 3765-3772.	1.2	6
31	Quantum transition probabilities during a perturbing pulse: Differences between the nonadiabatic results and Fermiâ€™s golden rule forms. Journal of Chemical Physics, 2018, 148, 194107.	1.2	6
32	The anisotropic polarizability of pairs of hydrogen molecules and the depolarized collision-induced roto-translational Raman light scattering spectra. Journal of Computational Methods in Sciences and Engineering, 2010, 10, 367-399.	0.1	4
33	Nonadiabatic transition probabilities in a time-dependent Gaussian pulse or plateau pulse: Toward experimental tests of the differences from Diracâ€™s transition probabilities. Journal of Chemical Physics, 2018, 149, 204110.	1.2	3
34	Variance of the energy of a quantum system in a time-dependent perturbation: Determination by nonadiabatic transition probabilities. Journal of Chemical Physics, 2020, 152, 104110.	1.2	3
35	Collision-Induced Infrared Absorption by Molecular Hydrogen Pairs at Thousands of Kelvin. International Journal of Spectroscopy, 2010, 2010, 1-11.	1.4	2
36	Collision-induced dipoles and polarizabilities of pairs of hydrogen molecules: Ab initio calculations and results from spherical tensor analysis. , 2012, , .		2

#	Article	IF	Citations
37	Ground and excited states of vanadium hydroxide isomers and their cations, VOH0,+ and HVO0,+. Journal of Chemical Physics, 2013, 138, 114305.	1.2	2
38	A single molecule as a dielectric medium. Journal of Chemical Physics, 2009, 131, 234303.	1.2	1
39	Collision-induced absorption at temperatures of thousands of kelvin, from first principles, for astrophysical applications. , 2010, , .		1
40	Response to â€œComment on â€˜Gauge-invariant expectation values of the energy of a molecule in an electromagnetic fieldâ€â€™ [J. Chem. Phys. 145, 147102 (2016)]. Journal of Chemical Physics, 2016, 145, 147103.	1.2	1
41	The interaction-induced dipole of H2â€“H: Newab initioresults and spherical tensor analysis. Journal of Chemical Physics, 2019, 150, 204307.	1.2	1
42	Bell inequalities for entangled qubits: quantitative tests of quantum character and nonlocality on quantum computers. Physical Chemistry Chemical Physics, 2021, 23, 6370-6387.	1.3	1
43	Quantum transition probabilities due to overlapping electromagnetic pulses: Persistent differences between Diracâ€™s form and nonadiabatic perturbation theory. Journal of Chemical Physics, 2021, 154, 024116.	1.2	1
44	Shannon and von Neumann entropies of multi-qubit SchrÃ¶dinger's cat states. Physical Chemistry Chemical Physics, 2022, 24, 7666-7681.	1.3	1
45	Infrared and vibrational raman band intensities: A new physical interpretation based on nonlocal polarizability densities. AIP Conference Proceedings, 1990, , .	0.3	0
46	Collision-induced changes in polarizability and raman scattering by atom-diatom pairs. AIP Conference Proceedings, 1990, , .	0.3	0
47	Derivatives of the polarization propagator including orbital relaxation effects. Journal of Chemical Physics, 2007, 126, 204105.	1.2	0
48	A Nonlocal Energy Functional Derived from the Fluctuation-Dissipation Theorem. ACS Symposium Series, 2007, , 169-182.	0.5	0