Markus SchrĶder

List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/6239557/publications.pdf Version: 2024-02-01



#	Article	IF	CITATIONS
1	Calculation of absorption spectra for light-harvesting systems using non-Markovian approaches as well as modified Redfield theory. Journal of Chemical Physics, 2006, 124, 084903.	3.0	104
2	Theoretical studies of the tunneling splitting of malonaldehyde using the multiconfiguration time-dependent Hartree approach. Journal of Chemical Physics, 2011, 134, 234307.	3.0	103
3	Calculation of the vibrational excited states of malonaldehyde and their tunneling splittings with the multi-configuration time-dependent Hartree method. Journal of Chemical Physics, 2014, 141, 034116.	3.0	50
4	Transforming high-dimensional potential energy surfaces into sum-of-products form using Monte Carlo methods. Journal of Chemical Physics, 2017, 147, 064105.	3.0	34
5	Transforming high-dimensional potential energy surfaces into a canonical polyadic decomposition using Monte Carlo methods. Journal of Chemical Physics, 2020, 152, 024108.	3.0	31
6	Realization of the CNOT quantum gate operation in six-dimensional ammonia using the OCT-MCTDH approach. Journal of Chemical Physics, 2009, 131, 034101.	3.0	30
7	Implementation of an iterative algorithm for optimal control of molecular dynamics into MCTDH. Physical Chemistry Chemical Physics, 2008, 10, 850-856.	2.8	25
8	Ab Initio Potential Energy and Dipole Moment Surfaces for CS ₂ : Determination of Molecular Vibrational Energies. Journal of Physical Chemistry A, 2013, 117, 6925-6931.	2.5	21
9	Generalized filtering of laser fields in optimal control theory: application to symmetry filtering of quantum gate operations. New Journal of Physics, 2009, 11, 105031.	2.9	18
10	Suitable coordinates for quantum dynamics: Applications using the multiconfiguration time-dependent Hartree (MCTDH) algorithm. Computational and Theoretical Chemistry, 2012, 990, 75-89.	2.5	18
11	High-Dimensional Quantum Dynamics Study on Excitation-Specific Surface Scattering Including Lattice Effects of a Five-Atom Surface Cell. Journal of Chemical Theory and Computation, 2021, 17, 2702-2713.	5.3	6
12	Absorption spectra for a model light-harvesting system using non-Markovian theories. Journal of Luminescence, 2005, 112, 461-464.	3.1	5
13	A Monte Carlo method for propagating multi-dimensional wave packets. Physica Status Solidi (B): Basic Research, 2004, 241, 2157-2167.	1.5	1
14	Vibrational Spectroscopy and Molecular Dynamics. Physical Chemistry in Action, 2014, , 117-145.	0.6	1
15	Representation of Diabatic Potential Energy Matrices for Multiconfiguration Time-Dependent Hartree Treatments of High-Dimensional Nonadiabatic Photodissociation Dynamics. Journal of Chemical Theory and Computation, 0, , .	5.3	1
16	Numerical Studies of the Tunneling Splitting of Malonaldehyde and the Eigenstates of Hydrated Hydroxide Anion Using MCTDH. , 2013, , 201-218.		0