Viktor Szalay

List of Publications by Year in descending order

32 papers	711 citations	687363 13 h-index	526287 27 g-index
32 all docs	32 docs citations	32 times ranked	426 citing authors

#	Article	IF	Citations
1	Discrete variable representations of differential operators. Journal of Chemical Physics, 1993, 99, 1978-1984.	3.0	91
2	The standard enthalpy of formation of CH2. Journal of Chemical Physics, 2003, 118, 10631-10642.	3.0	82
3	Variational vibrational calculations using high-order anharmonic force fields. Molecular Physics, 2004, 102, 2411-2423.	1.7	65
4	The generalized discrete variable representation. An optimal design. Journal of Chemical Physics, 1996, 105, 6940-6956.	3.0	62
5	Ab initiotorsional potential and transition frequencies of acetaldehyde. Journal of Chemical Physics, 2004, 120, 1203-1207.	3.0	48
6	On one-dimensional discrete variable representations with general basis functions. Journal of Chemical Physics, 2003, 119, 10512-10518.	3.0	39
7	Symmetry analysis of internal rotation. Journal of Chemical Physics, 2002, 117, 6489-6492.	3.0	37
8	Further extension of the Hougen-Bunker-Johns model. Journal of Molecular Spectroscopy, 1983, 102, 13-32.	1.2	27
9	Eckartâ^'Sayvetz conditions revisited. Journal of Chemical Physics, 2014, 140, 234107.	3.0	27
10	Derivation of the nonrigid rotation-large-amplitude internal motion Hamiltonian of the general molecule. Journal of Molecular Spectroscopy, 1988, 128, 24-61.	1.2	26
11	Adiabatic approximations to internal rotation. Journal of Chemical Physics, 2006, 124, 224310.	3.0	26
12	Iterative and direct methods employing distributed approximating functionals for the reconstruction of a potential energy surface from its sampled values. Journal of Chemical Physics, 1999, 111, 8804-8818.	3.0	23
13	Methanol as a Flexible Model. Journal of Molecular Spectroscopy, 1996, 180, 42-53.	1.2	18
14	The internal axis system of molecules with one large amplitude internal motion. Journal of Chemical Physics, 1998, 109, 3911-3918.	3.0	13
15	Finite basis representations with nondirect product basis functions having structure similar to that of spherical harmonics. Journal of Chemical Physics, 2006, 124, 014110.	3.0	12
16	A paradox of grid-based representation techniques: accurate eigenvalues from inaccurate matrix elements. Journal of Mathematical Chemistry, 2012, 50, 636-651.	1.5	12
17	Understanding nuclear motions in molecules: Derivation of Eckart frame ro-vibrational Hamiltonian operators via a gateway Hamiltonian operator. Journal of Chemical Physics, 2015, 142, 174107.	3.0	11
18	Determination of an isotope-independent puckering potential function of oxetane. Journal of Molecular Spectroscopy, 1987, 126, 1-12.	1.2	10

#	ARTICLE	IF	CITATIONS
19	Optimal grids for generalized finite basis and discrete variable representations: Definition and method of calculation. Journal of Chemical Physics, 2006, 125, 154115.	3.0	10
20	Vibrations of H+(D+) in stoichiometric LiNbO3 single crystal. Journal of Chemical Physics, 2011, 135, 124501.	3.0	9
21	On neglecting Coriolis and related couplings in first-principles rovibrational spectroscopy: Considerations of symmetry, accuracy, and simplicity. II. Case studies for H2O isotopologues, <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si886.svg"><mml:mrow><mml:msubsup><mml:mrow><mml:mtext>H</mml:mtext></mml:mrow><mml:mrow><mml:mn>3</mml:mn>	3.9	9
22	Rho-axis-system Hamiltonian for molecules with one large amplitude internal motion. Journal of Chemical Physics, 2003, 118, 6801-6805.	3.0	8
23	Application of contracted distributed approximating functions to solving vibrational eigenvalue problems. Journal of Chemical Physics, 1999, 110, 72-79.	3.0	7
24	Intelligent states for a number-operatorâ€“annihilation-operator uncertainty relation. Physical Review A, 2014, 89, .	2.5	7
25	Aspects of the Eckart frame ro-vibrational kinetic energy operator. Journal of Chemical Physics, 2015, 143, 064104.	3.0	6
26	The discrete variable representation of the rotational-vibrational Hamiltonian of triatomic molecules. Chemical Physics Letters, 1994, 231, 225-234.	2.6	5
27	Eckart ro-vibrational Hamiltonians via the gateway Hamilton operator: Theory and practice. Journal of Chemical Physics, 2017, 146, 124107.	3.0	5
28	Variational properties of the discrete variable representation: Discrete variable representation via effective operators. Journal of Chemical Physics, 2012, 137, 064118.	3.0	4
29	Internal- and rho-axis systems of molecules with one large amplitude internal motion: The geometry of rho. Journal of Chemical Physics, 2018, 149, 244118.	3.0	4
30	Derivation of rotational-vibrational Hamiltonian matrices of real elements. Molecular Physics, 1992, 75, 781-787.	1.7	3
31	Contracted distributed approximating functions: Derivation of non-oscillatory free particle and harmonic propagators for Feynman path integration in real time. Journal of Chemical Physics, 1998, 108, 2847-2866.	3.0	3
32	About the Variational Property of Generalized Discrete Variable Representation. Journal of Physical Chemistry A, 2013, 117, 7075-7080.	2.5	2