John Sabin

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Polarization Propagator Calculations. Advances in Quantum Chemistry, 1978, 11, 275-352.	0.8	338
2	Theoretical Investigation of the Electronic Structure and Properties of N3â^, N3, and N3+. Journal of Chemical Physics, 1971, 55, 1821-1829.	3.0	77
3	Theoretical stopping cross sections of Cî—,H, Cî—,C and C=C bonds for swift protons. Nuclear Instruments & Methods in Physics Research B, 1987, 27, 280-286.	1.4	52
4	Calculation of molecular mean excitation energies via the polarization propagator formalism:H2andH2O. Physical Review A, 1986, 34, 1104-1111.	2.5	50
5	Molecular shape, capacitance, and chemical hardness. International Journal of Quantum Chemistry, 2000, 77, 358-366.	2.0	50
6	On the applicability of LCAO-Xα methods to molecules containing transition metal atoms: The nickel atom and nickel hydride. International Journal of Quantum Chemistry, 1977, 12, 81-87.	2.0	42
7	Ab Initiocalculation of the vibrational and electronic properties of carbon dioxide. Journal of Chemical Physics, 1973, 59, 3003-3007.	3.0	30
8	Trajectory and molecular binding effects in stopping cross section for hydrogen beams on H2. Journal of Chemical Physics, 2002, 116, 2783-2793.	3.0	26
9	Hydrogen Bonds Involving Sulfur. II. The Hydrogen Sulfide–Hydrosulfide Complex. Journal of Chemical Physics, 1971, 54, 4675-4680.	3.0	25
10	SCF calculation of the effective parameters for the hubbard model of TCNQ charge-transfer salts. Molecular Physics, 1973, 26, 1177-1184.	1.7	23
11	Simulated structure and energetics of endohedral complexes of noble gas atoms in buckminsterfullerene. International Journal of Quantum Chemistry, 2007, 107, 3061-3066.	2.0	23
12	Dynamics of proton-acetylene collisions at 30 eV. Journal of Chemical Physics, 2002, 117, 1103-1108.	3.0	20
13	Polarization propagator calculation of spectroscopic properties of molecules. International Journal of Quantum Chemistry, 1991, 39, 371-386.	2.0	19
14	Mean Excitation Energies for Biomolecules. Advances in Quantum Chemistry, 2011, 62, 215-242.	0.8	18
15	Mean Excitation Energies and Energy Deposition Characteristics of Bio-organic Molecules. Journal of Physical Chemistry B, 2010, 114, 633-637.	2.6	16
16	Z-dependence of mean excitation energies for second and third row atoms and their ions. Journal of Chemical Physics, 2018, 148, 174307.	3.0	13
17	Coupled cluster calculations of mean excitation energies of the noble gas atoms He, Ne and Ar and of the H2molecule. Molecular Physics, 2014, 112, 751-761.	1.7	12
18	Mean excitation energies for molecular ions. Nuclear Instruments & Methods in Physics Research B, 2017, 394, 73-80.	1.4	12

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19	Shape-dependent molecular polarizabilities. International Journal of Quantum Chemistry, 2002, 86, 35-39.	2.0	11
20	Geometrical basis for molecular stopping anisotropy. Physical Review A, 1998, 58, 4616-4621.	2.5	10
21	Calculation of mean excitation energies. Advances in Quantum Chemistry, 2019, 80, 225-245.	0.8	10
22	Intermolecular potential studies of hydrogen-molecule interactions with rare-gas atoms. International Journal of Quantum Chemistry, 1976, 10, 213-221.	2.0	9
23	A semi-empirical investigation of the electronic structure and stability of the oxycumulenes. International Journal of Quantum Chemistry, 1973, 7, 261-267.	2.0	9
24	The influence of polarization functions on the directional. Molecular Physics, 1979, 37, 463-472.	1.7	8
25	Stopping power of molecules for fast ions. Molecular Physics, 2010, 108, 2891-2897.	1.7	8
26	Continuum Contributions to Dipole Oscillator-Strength Sum Rules for Hydrogen in Finite Basis Sets. Advances in Quantum Chemistry, 2017, 75, 229-241.	0.8	8
27	CNDO Study of the Properties of Ionic Defect Structure in a Model Oneâ€Dimensional Hydrogenâ€Bonded Chain. Journal of Chemical Physics, 1972, 56, 45-51.	3.0	7
28	Prediction of crystalline properties from ultrathin layered systems: Energy deposition. International Journal of Quantum Chemistry, 1995, 56, 153-159.	2.0	6
29	Test of the validity of Bragg's rule for mean excitation energies of small molecules and ions. Nuclear Instruments & Methods in Physics Research B, 2019, 444, 112-116.	1.4	6
30	Excited electronic states of a hydrogen bond: Bifluoride ion. International Journal of Quantum Chemistry, 1979, 16, 273-275.	2.0	5
31	Amino Acid Mean Excitation Energies and Directional Dependencies from Core and Bond Calculations. , 2008, , .		5
32	The quadrupole polarizability and spectral moments of the quadrupole oscillator strength distribution of N2. Molecular Physics, 1991, 72, 1267-1284.	1.7	4
33	An analytical representation of shell corrections for stopping power. International Journal of Quantum Chemistry, 2009, 109, 2933-2936.	2.0	4
34	Fewâ€parameter exponentially correlated wavefunctions for the ground state of lithium. International Journal of Quantum Chemistry, 2009, 109, 3791-3797.	2.0	4
35	Calculation of mean excitation energies of 3d-elements and their cations. Molecular Physics, 2021, 119, e1823508.	1.7	4
36	Generalized oscillator strengths for calculation of molecular stopping properties, some preliminary results: Co. , 1997, , .		2

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37	Bond correction factors and their applications to the calculation of molecular mean excitation energies. Nuclear Instruments & Methods in Physics Research B, 2020, 468, 28-36.	1.4	2
38	Molecular shape, capacitance, and chemical hardness. International Journal of Quantum Chemistry, 2000, 77, 358.	2.0	2
39	Simulations of Xe@C ₆₀ collisions with graphitic films. International Journal of Quantum Chemistry, 2008, 108, 3010-3015.	2.0	1
40	A comment concerning SHS type hydrogen bonds. International Journal of Quantum Chemistry, 1971, 5, 133-136.	2.0	1
41	A CNDO estimate of the relative affinities of taurine and isethionic acid for alkali metal ions. International Journal of Quantum Chemistry, 1974, 8, 43-48.	2.0	1
42	Ab Initio calculation of some electronically excited states of a hydrogen-bonded system: A preliminary report. International Journal of Quantum Chemistry, 1975, 9, 259-262.	2.0	1
43	From Stopping Power to Radiation Dose Equivalent: Views of the Interaction of Swift Ions with Matter. , 2008, , .		0
44	Localized electronic excitation in a hydrogen bond. International Journal of Quantum Chemistry, 2009, 22, 289-296.	2.0	0
45	On the orbital implementation of the kinetic theory of stopping. International Journal of Quantum Chemistry, 1989, 36, 557-563.	2.0	0
46	Electron distribution in a short a-type hydrogen bond. International Journal of Quantum Chemistry, 2009, 6, 301-304.	2.0	0
47	Oscillatory behaviour of charge transfer probabilities in ion-atom collisions. Molecular Physics, 2012, 110, 561-563.	1.7	0
48	On the relationship between bond correction factors and elemental mean excitation energies. Nuclear Instruments & Methods in Physics Research B, 2020, 474, 6-9.	1.4	0