Daniel K W Mok

List of Publications by Year
in descending order

52 papers	1,223 citations	471061 17 h-index	377514 34 g-index
52 all docs	52 docs citations	52 times ranked	1132 citing authors

#	Article	IF	Citations
1	Comment on â€œImpact of water on the BrO + HO2 gas-phase reaction: mechanism, kinetics and productsâ€• by N. T. Tsona, S. Tang and L. Du, Phys. Chem. Chem. Phys., 2019, 21, 20296. Physical Chemistry Chemical Physics, 2021, 23, 6309-6315.	1.3	1
2	Schwann cell-specific Pten inactivation reveals essential role of the sympathetic nervous system activity in adipose tissue development. Biochemical and Biophysical Research Communications, 2020, 531, 118-124.	1.0	2
3	A theoretical study of the addition of CH₂OO to hydroxymethyl hydroperoxide and its implications on SO₃ formation in the atmosphere. Physical Chemistry Chemical Physics, 2020, 22, 14130-14141.	1.3	2
4	HBx-K130M/V131I Promotes Liver Cancer in Transgenic Mice via AKT/FOXO1 Signaling Pathway and Arachidonic Acid Metabolism. Molecular Cancer Research, 2019, 17, 1582-1593.	1.5	29
5	The Atmospherically Important Reaction of Hydroxyl Radicals with Methyl Nitrate: A Theoretical Study Involving the Calculation of Reaction Mechanisms, Enthalpies, Activation Energies, and Rate Coefficients. Journal of Physical Chemistry A, 2017, 121, 6554-6567.	1.1	5
6	Direct Measurements of Unimolecular and Bimolecular Reaction Kinetics of the Criegee Intermediate (CH₃)₂COO. Journal of Physical Chemistry A, 2017, 121, 4-15.	1.1	87
7	Simulation of the photodetachment spectrum of HHfOâ¯ using coupled-cluster calculations. Journal of Chemical Physics, 2016, 145, 244303.	1.2	0
8	Simulation of the single-vibronic-level emission spectra of HAsO and DAsO. Journal of Chemical Physics, 2016, 144, 184303.	1.2	6
9	A Study of H₂O₂ with Threshold Photoelectron Spectroscopy (TPES) and Electronic Structure Calculations: Redetermination of the First Adiabatic Ionization Energy (AIE). Journal of Physical Chemistry A, 2016, 120, 5220-5229.	1.1	5
10	A theoretical study of the atmospherically important radicalâ€“radical reaction BrO + HO₂; the product channel O₂(a¹Î”_g) + HOBr is formed with the highest rate. Physical Chemistry Chemical Physics, 2016, 18, 30554-30569.	1.3	10
11	Reaction between CH₃O₂ and BrO Radicals: A New Source of Upper Troposphere Lower Stratosphere Hydroxyl Radicals. Journal of Physical Chemistry A, 2015, 119, 4618-4632.	1.1	18
12	A theoretical study of the mechanism of the atmospherically relevant reaction of chlorine atoms with methyl nitrate, and calculation of the reaction rate coefficients at temperatures relevant to the troposphere. Physical Chemistry Chemical Physics, 2015, 17, 7463-7476.	1.3	3
13	Simulation of the single-vibronic-level emission spectrum of HPS. Journal of Chemical Physics, 2014, 140, 194311.	1.2	7
14	Petroleum ether extractive of the hips of Rosa multiflora ameliorates collagen-induced arthritis in rats. Journal of Ethnopharmacology, 2014, 157, 45-54.	2.0	28
15	Rate Coefficients of the Cl + CH₃C(O)OCH₃ â†' HCl + CH₃C(O)OCH₂ Reaction at Different Temperatures Calculated by Transition-State Theory with ab Initio and Density Functional Theory Reaction Paths. Journal of Physical Chemistry A, 2014, 118, 2040-2055.	1.1	17
16	Direct Measurements of Conformer-Dependent Reactivity of the Criegee Intermediate CH ₃ CHOO. Science, 2013, 340, 177-180.	6.0	379
17	Rate coefficients of the CF₃CHFCF₃ + H â†' CF₃CFCF₃ + H₂ reaction at different temperatures calculated by transition state theory with ab initio and DFT reaction paths. Journal of Computational Chemistry, 2013, 34, 545-557.	1.5	18
18	Simulated photodetachment spectra of AlH2â¯. Journal of Chemical Physics, 2013, 139, 014301.	1.2	5

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19	Spectroscopy of the Simplest Criegee Intermediate CH₂OO: Simulation of the First Bands in Its Electronic and Photoelectron Spectra. Chemistry - A European Journal, 2012, 18, 12411-12423.	1.7	54
20	The enthalpies of formation of AsXn molecules, where X = H, F or Cl, and n = 1, 2 or 3, by RCCSD(T) and UCCSD(T)-F12x calculations. Physical Chemistry Chemical Physics, 2011, 13, 9540.	1.3	15
21	Anti-inflammatory activities and mechanisms of action of the petroleum ether fraction of Rosa multiflora Thunb. hips. Journal of Ethnopharmacology, 2011, 138, 717-722.	2.0	44
22	Franckâ€“Condon simulation of the photoelectron spectrum of AsCl₂ and the photodetachment spectrum of AsCl employing UCCSD(T)â€F12a potential energy functions: IE and EA of AsCl₂. Journal of Computational Chemistry, 2011, 32, 1648-1660.	1.5	3
23	Franck-Condon simulation, including anharmonicity, of the photodetachment spectrum of P2Hâ^: Restricted-spin coupled-cluster single-double plus perturbative triple and unrestricted-spin coupled-cluster single-double plus perturbative triple -F12x potential energy functions of P2H and P2Hâ^. Journal of Chemical Physics, 2011, 135, 124312.	1.2	3
24	Highâ€level ab initio calculations on HGeCl and the equilibrium geometry of the Ãƒ¹Aâ€³ state derived from Franckâ€Condon analysis of the singleâ€vibronicâ€level emission spectra of HGeCl and DGeCl. Journal of Computational Chemistry, 2010, 31, 476-491.	1.5	5
25	Ab initio calculations on the XÌƒâ€‰B21 and AÌƒâ€‰A21 states of AsH2, and Franckâ€“Condon simulation, including anharmonicity, of the AÌƒ(0,0,0)-XÌƒ single vibronic level emission spectrum of AsH2. Journal of Chemical Physics, 2010, 132, 234309.	1.2	9
26	Franckâ€“Condon simulation of the photoelectron spectrum of AsF2 and the photodetachment spectrum of AsF2â^ using ab initio calculations: Ionization energy and electron affinity of AsF2. Physical Chemistry Chemical Physics, 2010, 12, 9075.	1.3	5
27	A combined ab initio and Franckâ€Condon factor simulation study on the photodetachment spectrum of ScO₂^{â^}. Journal of Computational Chemistry, 2009, 30, 337-345.	1.5	10
28	Difluorocarbene Studied with Threshold Photoelectron Spectroscopy (TPES): Measurement of the First Adiabatic Ionization Energy (AIE) of CF₂. Chemistry - A European Journal, 2008, 14, 11452-11460.	1.7	23
29	Ab initio calculations on low-lying electronic states of SnCl₂^{â^}and Franckâ€“Condon simulation of its photodetachment spectrum. Physical Chemistry Chemical Physics, 2008, 10, 834-843.	1.3	4
30	A combined ab initio and Franckâ€“Condon factor simulation study on the photodetachment spectrum of HfO2â^. Physical Chemistry Chemical Physics, 2008, 10, 7270.	1.3	7
31	An Ab Initio Study of the Low-Lying Electronic States of YO₂ and Franckâ^Condon Simulation of the First Photodetachment Band of YO₂^{â^}. Journal of Physical Chemistry A, 2008, 112, 4511-4520.	1.1	14
32	Ab initiocalculations on SnCl2 and Franck-Condon factor simulations of its aÌƒ-XÌƒ and BÌƒ-XÌƒ absorption and single-vibronic-level emission spectra. Journal of Chemical Physics, 2007, 127, 024308.	1.2	6
33	Ab initio calculations on low-lying electronic states of SbO2â^ and Franck-Condon simulation of its photodetachment spectrum. Journal of Chemical Physics, 2007, 127, 094306.	1.2	2
34	Ab initio calculations on the XÌƒAâ€²1 and AÌƒAâ€³1 states of HPO and Franck-Condon simulation of the single vibronic level emission spectra of HPO and DPO. Journal of Chemical Physics, 2007, 127, 214305.	1.2	10
35	Ab Initio Study of Low-Lying Electronic States of SnCl2+. Journal of Physical Chemistry A, 2007, 111, 13193-13199.	1.1	5
36	DFT and ab initio calculations on two reactions between hydrogen atoms and the fire suppressants 2-H heptafluoropropane and CF3 Br. Journal of Computational Chemistry, 2007, 28, 1582-1592.	1.5	14

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37	Ab initiocalculations on SCl2 and low-lying cationic states of SCl2+: Franck-Condon simulation of the UV photoelectron spectrum of SCl2. Journal of Chemical Physics, 2006, 125, 104303.	1.2	6
38	Ab initio calculations on SF2 and its low-lying cationic states: Anharmonic Franck-Condon simulation of the uv photoelectron spectrum of SF2. Journal of Chemical Physics, 2006, 125, 104304.	1.2	6
39	An ab initio study on the ground and low-lying doublet electronic states of SbO2. Journal of Chemical Physics, 2006, 125, 064307.	1.2	6
40	Ab Initio Calculations and Franck-Condon Simulation of the Absorption Spectra of GeCl2 Including Anharmonicity. ChemPhysChem, 2005, 6, 719-731.	1.0	9
41	The Singlet-Triplet Separation in CF2: State-of-the-Art Ab Initio Calculations and Franck-Condon Simulations Including Anharmonicity. ChemPhysChem, 2005, 6, 2037-2045.	1.0	28
42	A Combined Ab Initio/Franck-Condon Study of the Ãƒ-?? Single-Vibronic-Level Emission Spectrum of CCl2 and the Photodetachment Spectrum of CCl2â¯. ChemPhysChem, 2005, 6, 2046-2059.	1.0	28
43	Use of the ultraviolet absorption spectrum of CF2 to determine the spatially resolved absolute CF2 density, rotational temperature, and vibrational distribution in a plasma etching reactor. Journal of Chemical Physics, 2004, 120, 9499-9508.	1.2	35
44	Franckâ€“Condon simulation of the single vibronic level emission spectra of HSiF and DSiF including anharmonicity. Journal of Chemical Physics, 2004, 120, 1292-1305.	1.2	26
45	Franck-Condon simulation of the single-vibronic-level emission spectra of HPCl/DPCl and the chemiluminescence spectrum of HPCl, including anharmonicity. Journal of Chemical Physics, 2004, 121, 1810-1823.	1.2	13
46	Ab initio calculations on low-lying electronic states of TeO2 and Franck-Condon simulation of the (1)1B2â†Xìƒâ€Š1A1 TeO2 absorption spectrum including anharmonicity. Journal of Chemical Physics, 2004, 121, 2962-2974.	1.2	12
47	Ab Initio Calculations on PO2 and Anharmonic Franckâ¯Condon Simulations of Its Single-Vibrational-Level Emission Spectra. Journal of Physical Chemistry A, 2002, 106, 10130-10138.	1.1	20
48	Ab Initio Calculations on the (1)2Î" Excited State and Low-Lying Quartet States of GaÂ·N2:Â Simulation of Its LIF Spectrum. Journal of Physical Chemistry A, 2001, 105, 9533-9542.	1.1	9
49	Ab initio calculations on the and states of AlNC and simulation of the AlNC- emission spectra. Journal of Computational Chemistry, 2001, 22, 1896-1906.	1.5	8
50	Simulation of Ãƒâ€Š1B1â†'Xìƒâ€Š1A1 CF2 single vibronic level emissions: Including anharmonic and Duschinsky effects. Journal of Chemical Physics, 2001, 115, 5816-5822.	1.2	40
51	A new method of calculation of Franckâ€“Condon factors which includes allowance for anharmonicity and the Duschinsky effect: Simulation of the Heâ€‰I photoelectron spectrum of ClO2. Journal of Chemical Physics, 2000, 113, 5791-5803.	1.2	103
52	Xìƒ1A1, Ã£3B1, and Ãƒ1B1States of SiCl2:Â Ab Initio Calculations and Simulation of Emission Spectra. Journal of Physical Chemistry A, 1999, 103, 4925-4932.	1.1	19