AntÃ³nio J C Varandas

List of Publications by Year
in descending order

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409	10,889	36303	69250
papers	citations	51 h-index	77 g-index

421	421	421	3150
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A double manyâ€body expansion of the two lowestâ€energy potential surfaces and nonadiabatic coupling for H3. Journal of Chemical Physics, 1987, 86, 6258-6269.	3.0	373
2	Analytical potentials for triatomic molecules from spectroscopic data. Molecular Physics, 1976, 32, 1359-1372.	1.7	249
3	Recalibration of a single-valued double many-body expansion potential energy surface for ground-state hydroperoxy and dynamics calculations for the oxygen atom + hydroxyl .fwdarw. oxygen + hydrogen atom reaction. The Journal of Physical Chemistry, 1990, 94, 8073-8080.	2.9	244
4	Predicting Catalysis:Â Understanding Ammonia Synthesis from First-Principles Calculations. Journal of Physical Chemistry B, 2006, 110, 17719-17735.	2.6	192
5	Extrapolating to the one-electron basis-set limit in electronic structure calculations. Journal of Chemical Physics, 2007, 126, 244105.	3.0	176
6	Intermolecular and Intramolecular Potentials: Topographical Aspects, Calculation, and Functional Representation via A Double Many-Body Expansion Method. Advances in Chemical Physics, 2007, , 255-338.	0.3	160
7	Basis-set extrapolation of the correlation energy. Journal of Chemical Physics, 2000, 113, 8880-8887.	3.0	151
8	A realistic double many-body expansion (DMBE) potential energy surface for ground-state O3from a multiproperty fit toab initiocalculations, and to experimental spectroscopic, inelastic scattering, and kinetic isotope thermal rate data. Molecular Physics, 1988, 65, 843-860.	1.7	138
9	Quasiclassical trajectory calculations of the thermal rate coefficients for the reactions H(D)+O2â†'OH(D)+O and O+OH(D)â†'O2+H(D) as a function of temperature. Journal of Chemical Physics, 1992, 96, 5137-5150.	3.0	125
10	Potential model for diatomic molecules including the united-atom limit and its use in a multiproperty fit for argon. Journal of the Chemical Society, Faraday Transactions, 1992, 88, 941.	1.7	122
11	Excitation function for H+O2 reaction: A study of zeroâ€point energy effects and rotational distributions in trajectory calculations. Journal of Chemical Physics, 1993, 99, 1076-1085.	3.0	120
12	A novel non-active model to account for the leak of zero-point energy in trajectory calculations. Application to H + O2 reaction near threshold. Chemical Physics Letters, 1994, 225, 18-27.	2.6	113
13	Energy switching approach to potential surfaces: An accurate singleâ€valued function for the water molecule. Journal of Chemical Physics, 1996, 105, 3524-3531.	3.0	111
14	A general approach to the potential energy functions of small polyatomic systems: Molecules and van der Waals molecules. Computational and Theoretical Chemistry, 1985, 120, 401-424.	1.5	100
15	Quantum mechanical valence study of a bond-breaking-bond-forming process in triatomic systems. International Journal of Quantum Chemistry, 1994, 52, 1153-1176.	2.0	100
16	A many-body expansion of polyatomic potential energy surfaces: application to H n systems. Faraday Discussions of the Chemical Society, 1977, 62, 92.	2.2	96
17	A useful triangular plot of triatomic potential energy surfaces. Chemical Physics Letters, 1987, 138, 455-461.	2.6	89
18	Use of scaled external correlation, a double manyâ€body expansion, and variational transition state theory to calibrate a potential energy surface for FH2. Journal of Chemical Physics, 1991, 94, 7136-7149.	3.0	89

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19	Analytical potentials for triatomic molecules. Molecular Physics, 1982, 45, 1053-1066.	1.7	87
20	A realistic hydroperoxo(~X2A") potential energy surface from the double many-body expansion method. The Journal of Physical Chemistry, 1988, 92, 3732-3742.	2.9	83
21	A semiempirical method for correcting configuration interaction potential energy surfaces. Journal of Chemical Physics, 1989, 90, 4379-4391.	3.0	83
22	Four-atom bimolecular reactions with relevance in environmental chemistry: Theoretical work. International Reviews in Physical Chemistry, 2000, 19, 199-245.	2.3	82
23	Accurate ab initio based multisheeted double many-body expansion potential energy surface for the three lowest electronic singlet states of H3+. Journal of Chemical Physics, 2007, 126, 074309.	3.0	81
24	Narrowing the error in electron correlation calculations by basis set re-hierarchization and use of the unified singlet and triplet electron-pair extrapolation scheme: Application to a test set of 106 systems. Journal of Chemical Physics, 2014, 141, 224113.	3.0	76
25	Accurate DMBE Potential Energy Surface For the N(2D) + H2(1Î£ g +) Reaction Using an Improved Switching Function Formalism. Theoretical Chemistry Accounts, 2006, 116, 404-419.	1.4	73
26	On the relation of dispersion to induction energies, and to their damping functions. Molecular Physics, 1987, 60, 527-539.	1.7	70
27	Extrapolation to the Complete Basis Set Limit without Counterpoise. The Pair Potential of Helium Revisited^{â€}. Journal of Physical Chemistry A, 2010, 114, 8505-8516.	2.5	69
28	Chercher le croisement. Chemical Physics Letters, 1979, 61, 431-434.	2.6	68
29	A Quantum Wave Packet Dynamics Study of the N(2D) + H2Reactionâ€. Journal of Physical Chemistry A, 2006, 110, 1666-1671.	2.5	68
30	A simple semi-empirical approach to the intermolecular potential of van der Waals systems. Molecular Physics, 1982, 45, 857-875.	1.7	67
31	Method for quasiclassical trajectory calculations on potential energy surfaces defined from gradients and Hessians, and model to constrain the energy in vibrational modes. Journal of Chemical Physics, 1994, 100, 1908-1920.	3.0	66
32	Straightening the Hierarchical Staircase for Basis Set Extrapolations: A Low-Cost Approach to High-Accuracy Computational Chemistry. Annual Review of Physical Chemistry, 2018, 69, 177-203.	10.8	65
33	Single-Valued DMBE Potential Energy Surface for HSO:Â A Distributedn-Body Polynomial Approach. Journal of Physical Chemistry A, 2001, 105, 5923-5932.	2.5	64
34	Towards a double many-body expansion method for multivalued potential energy surfaces. Molecular Physics, 1995, 85, 497-526.	1.7	63
35	Ab initio theoretical calculation and potential energy surface for ground-state HO3. Chemical Physics Letters, 2001, 334, 173-178.	2.6	63
36	Accurate ab initio potential energy curves for the classic Liâ€“F ionic-covalent interaction by extrapolation to the complete basis set limit and modeling of the radial nonadiabatic coupling. Journal of Chemical Physics, 2009, 131, 124128.	3.0	62

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37	A new formulation of three-body dynamical correlation energy for explicit potential functions. Chemical Physics Letters, 1992, 194, 333-340.	2.6	61
38	Trajectory binning scheme and non-active treatment of zero-point energy leakage in quasi-classical dynamics. Chemical Physics Letters, 2007, 439, 386-392.	2.6	60
39	Extrapolation to the complete-basis-set limit and the implications of avoided crossings: The Xâ€‰Î£1g+, Bâ€‰Î”1g, and Bâ€²â€‰Î£1g+ states of C2. Journal of Chemical Physics, 2008, 129, 234103.	3.0	60
40	Implications of the O + OH reaction in hydroxyl nightglow modeling. Atmospheric Chemistry and Physics, 2013, 13, 1-13.	4.9	60
41	Analytical potentials for triatomic molecules from spectroscopic data. Molecular Physics, 1977, 34, 947-962.	1.7	59
42	Reaction rates of H(H2), D(H2), and H(D2) van der Waals molecules and the threshold behavior of the bimolecular gasâ€phase rate coefficient. Journal of Chemical Physics, 1989, 91, 3492-3503.	3.0	59
43	Hartreeâ€“Fock approximate correlation energy (HFACE) potential for diatomic interactions. Molecules and van der Waals molecules. Journal of the Chemical Society, Faraday Transactions 2, 1986, 82, 593-608.	1.1	58
44	A double many-body expansion of molecular potential energy functions. Molecular Physics, 1986, 57, 387-414.	1.7	57
45	A double many-body expansion of molecular potential energy functions. Molecular Physics, 1984, 53, 1303-1325.	1.7	56
46	Double many-body expansion potential energy surface for ground state HSO2. Physical Chemistry Chemical Physics, 2005, 7, 2305.	2.8	56
47	Double many-body expansion potential energy surface for ground-state HCN based on realistic long range forces and accurateab initiocalculations. Journal of Chemical Physics, 1997, 106, 9647-9658.	3.0	55
48	A general inter-relationship between transition-state bond extensions and the energy barrier to reaction. Journal of the Chemical Society, Faraday Transactions 2, 1986, 82, 953.	1.1	54
49	On the chaperon mechanism for association rate constants: the formation of HO2 and O3. Chemical Physics Letters, 1996, 249, 264-271.	2.6	53
50	A detailed stateâ€toâ€state lowâ€energy dynamics study of the reaction O(3P)+OH(2Î)â†'O2(XÌƒâ€‰3Î£gâ^')+H(2S) using a quasiclassical trajectoryâ€“internalâ€energy quantumâ€mechanicalâ€threshold method. Journal of Chemical Physics, 1992, 97, 4050-4065.	3.0	52
51	Quasiclassical trajectory calculations of the thermal rate coefficient for the oxygen atom + hydroxyl .fwdarw. oxygen + hydrogen atom reaction on realistic double many-body expansion potential energy surfaces for ground-state hydroperoxy. The Journal of Physical Chemistry, 1988, 92, 4552-4555.	2.9	51
52	Accurate Double Many-Body Expansion Potential Energy Surface for N₃(⁴Aâ€²â€²) from Correlation Scaled ab Initio Energies with Extrapolation to the Complete Basis Set Limit. Journal of Physical Chemistry A, 2009, 113, 14424-14430.	2.5	51
53	Dynamics of the 18O + 16O2(Ï…=0) exchange reaction on a new potential energy surface for ground-state ozone. Chemical Physics Letters, 1982, 88, 1-6.	2.6	50
54	On phase factors and geometric phases in isotopes of H3: A line integral study. Journal of Chemical Physics, 2000, 112, 2746-2751.	3.0	50

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55	Unimolecular and Bimolecular Calculations for HN2. Journal of Physical Chemistry A, 2005, 109, 2356-2363.	2.5	50
56	Accurate ab initio double many-body expansion potential energy surface for ground-state H2S by extrapolation to the complete basis set limit. Journal of Chemical Physics, 2009, 130, 134317.	3.0	50
57	Energy switching approach to potential surfaces. II. Two-valued function for the water molecule. Journal of Chemical Physics, 1997, 107, 867-878.	3.0	49
58	Dynamics of H(D)+O3 reactions on a double many-body expansion potential-energy surface for ground state HO3. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 2651-2656.	1.7	48
59	Semiclassical variational transition state calculations for the reactions of H and D with thermal and vibrationally excited H2. International Journal of Chemical Kinetics, 1986, 18, 1065-1077.	1.6	47
60	Accurate global ab initio potentials at low-cost by correlation scaling and extrapolation to the one-electron basis set limit. Chemical Physics Letters, 2007, 443, 398-407.	2.6	47
61	Nuclear dynamics in the vicinity of the crossing seam: Theory and application to vibrational spectrum of H3. Journal of Chemical Physics, 2000, 112, 2121-2127.	3.0	46
62	A realistic multi-sheeted potential energy surface for NO2(2Aâ€²) from the double many-body expansion method and a novel multiple energy-switching scheme. Journal of Chemical Physics, 2003, 119, 2596-2613.	3.0	46
63	OH(v)+O3: Does chemical reaction dominate over non-reactive quenching?. Chemical Physics Letters, 2001, 340, 62-70.	2.6	45
64	Accurate ab initio potentials at low cost via correlation scaling and extrapolation: Application to CO(AÎ1). Journal of Chemical Physics, 2007, 127, 114316.	3.0	45
65	HN₂(²Aâ€˜) Electronic Manifold. II. Ab Initio Based Double-Sheeted DMBE Potential Energy Surface via a Global Diabatization Angle. Journal of Physical Chemistry A, 2008, 112, 3768-3786.	2.5	45
66	Ab Initio Treatment of Bond-Breaking Reactions: Accurate Course of HO₃ Dissociation and Revisit to Isomerization. Journal of Chemical Theory and Computation, 2012, 8, 428-441.	5.3	45
67	Perturbation calculations of rare-gas potentials near the van der Waals minimum. Molecular Physics, 1975, 30, 223-236.	1.7	44
68	Repulsive double many-body expansion potential energy surface for the reactions N(4S)+ H2â‡Œ NH(X3Î£â€“)+ H from accurate ab initio calculations. Physical Chemistry Chemical Physics, 2005, 7, 2867.	2.8	44
69	Nonadiabatic effects in D++H2 and H++D2. Chemical Physics Letters, 2009, 471, 222-228.	2.6	44
70	New Double Many-Body Expansion Potential Energy Surface for Ground-State HCN from a Multiproperty Fit to Accurate ab Initio Energies and Rovibrational Calculationsâ€. Journal of Physical Chemistry A, 2006, 110, 485-493.	2.5	43
71	Nonadiabatic effects in the H+D2 reaction. Journal of Chemical Physics, 2006, 125, 133108.	3.0	43
72	Geometric phase effects on transition-state resonances and bound vibrational states of H3 via a time-dependent wavepacket method. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 819-824.	1.7	42

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73	Bound Ro-Vibronic States of TripletH3+. Physical Review Letters, 2001, 86, 1183-1186.	7.8	42
74	On the O2(Î½â€²) + O2(Î½â€²) atmospheric reaction: a quasiclassical trajectory study. Chemical Physics, 1997, 215, 167-182.	1.9	41
75	Accurate rate constant and quantum effects for N(2D)+H2 reaction. Chemical Physics Letters, 2006, 421, 415-420.	2.6	41
76	Reactive and non-reactive vibrational quenching in O + OH collisions. Chemical Physics Letters, 2004, 396, 182-190.	2.6	40
77	Can extrapolation to the basis set limit be an alternative to the counterpoise correction? A study on the helium dimer. Theoretical Chemistry Accounts, 2008, 119, 511-521.	1.4	40
78	Generalized Uniform Singlet- and Triplet-Pair Extrapolation of the Correlation Energy to the One Electron Basis Set Limit. Journal of Physical Chemistry A, 2008, 112, 1841-1850.	2.5	40
79	Double many-body expansion of molecular potential energy functions and the role of long-range forces in the rates of chemical reactions. Computational and Theoretical Chemistry, 1988, 166, 59-74.	1.5	39
80	Are Vibrationally Excited Molecules a Clue for the â€œO3Deficit Problemâ€•and â€œHOxDilemmaâ€•in the Middle Atmosphere?. Journal of Physical Chemistry A, 2004, 108, 758-769.	2.5	39
81	Quasi-classical trajectory and quantum mechanics study of the reaction H(2S)+NHâ†'N(4S)+H2. Chemical Physics Letters, 2010, 493, 225-228.	2.6	39
82	Test studies on the potential energy surface and rate constant for the OH+O3 atmospheric reaction. Chemical Physics Letters, 2000, 331, 474-482.	2.6	38
83	Accurate Single-Valued Double Many-Body Expansion Potential Energy Surface for Ground-State HN2. Journal of Physical Chemistry A, 2003, 107, 7923-7930.	2.5	38
84	Dynamics of X+CH4 (X=H,O,Cl) reactions: How reliable is transition state theory for fine-tuning potential energy surfaces?. Journal of Chemical Physics, 2006, 125, 064312.	3.0	38
85	Double many-body expansion potential energy surface for ground-state HO3. Molecular Physics, 1997, 91, 301-318.	1.7	37
86	Existence of strictly diabatic basis sets for the two-state problem. International Journal of Quantum Chemistry, 2002, 89, 255-259.	2.0	37
87	On the stability of the elusive HO3 radical. Physical Chemistry Chemical Physics, 2011, 13, 15619.	2.8	37
88	A LEPS potential for H3 from force field data. Journal of Chemical Physics, 1979, 70, 3786-3795.	3.0	36
89	Threeâ€dimensional quantum mechanical rate constants for the reaction O+O3â†'2O2, employing a sixâ€dimensional potential energy surface. Journal of Chemical Physics, 1995, 102, 3474-3476.	3.0	36
90	Dynamics of HO2+O3 reaction using a test DMBE potential energy surface: does it occur via oxygen or hydrogen atom abstraction?. Chemical Physics Letters, 2004, 385, 409-416.	2.6	36

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91	Dynamics Study of the N(4S) + O2Reaction and Its Reverse. Journal of Physical Chemistry A, 2004, 108, 3556-3564.	2.5	36
92	Combined-hyperbolic-inverse-power-representation of potential energy surfaces: A preliminary assessment for H3 and HO2. Journal of Chemical Physics, 2013, 138, 054120.	3.0	36
93	Accurate combined-hyperbolic-inverse-power-representation of ab initio potential energy surface for the hydroperoxyl radical and dynamics study of $f O+OH$O+OH reaction. Journal of Chemical Physics, 2013, 138, 134117.	3.0	36
94	Calculation of the asymptotic interaction and modelling of the potential energy curves of OH and OH+. Chemical Physics, 1995, 194, 91-100.	1.9	35
95	Cross sections and rate constants for the O(1D) + H2 reaction using a single-valued energy-switching potential energy surface. Chemical Physics Letters, 1997, 278, 325-332.	2.6	35
96	Theoretical study of the reaction OH+SOâ†'H+SO2. Chemical Physics Letters, 2007, 433, 279-285.	2.6	35
97	Is HO3 minimum cis or trans? An analytic full-dimensional ab initio isomerization path. Physical Chemistry Chemical Physics, 2011, 13, 9796.	2.8	35
98	The coupled 3D wave packet approach for triatomic reactive scattering in hyperspherical coordinates. Computer Physics Communications, 2013, 184, 270-283.	7.5	35
99	A realistic double many-body expansion potential energy surface for from a multiproperty fit to accurate ab initio energies and vibrational levels. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2002, 58, 629-647.	3.9	34
100	Benchmarking of Density Functionals for the Accurate Description of Thiolâ€"Disulfide Exchange. Journal of Chemical Theory and Computation, 2014, 10, 4842-4856.	5.3	33
101	Analytical potentials for triatomic molecules from spectroscopic data. Molecular Physics, 1978, 35, 1325-1336.	1.7	32
102	Theoretical 3D study of transition state resonances for the H + H2 reaction using two coupled diabatic potential energy surfaces. Chemical Physics Letters, 1996, 259, 336-341.	2.6	32
103	Energy switching approach to potential surfaces. III. Three-valued function for the water molecule. Journal of Chemical Physics, 1998, 108, 7623-7630.	3.0	32
104	On the â€œOzone Deficit Problemâ€• What Are Ox and HOx Catalytic Cycles for Ozone Depletion Hiding?. ChemPhysChem, 2002, 3, 433.	2.1	32
105	Application of renormalized coupled-cluster methods to potential function of water. Theoretical Chemistry Accounts, 2008, 120, 59-78.	1.4	32
106	Extrapolating potential energy surfaces by scaling electron correlation at a single geometry. Chemical Physics Letters, 2006, 430, 448-453.	2.6	31
107	Choosing points in potential energy surfaces for fitting polynomial functions: application of permutational symmetry. Chemical Physics Letters, 1981, 84, 440-445.	2.6	30
108	Thermophysical Properties of Alkali Metal Vapours, Part I â€" Theoretical Calculation of the Properties of Monatomic Systems. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1990, 94, 53-59.	0.9	30

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109	Atom-molecule dispersion-energy coefficients and their dependence on the intramolecular coordinate: A-H2systems. Molecular Physics, 1990, 70, 623-644.	1.7	30
110	Accurate MRCI study of ground-state N2H2 potential energy surface. Chemical Physics Letters, 2006, 424, 46-53.	2.6	30
111	Accurate Double Many-Body Expansion Potential Energy Surface for Ground-State HS₂Based on ab Initio Data Extrapolated to the Complete Basis Set Limit. Journal of Physical Chemistry A, 2011, 115, 5274-5283.	2.5	30
112	Semi-empirical valence bond potential energy surfaces for homonuelear alkali trimers. Molecular Physics, 1982, 47, 1241-1251.	1.7	29
113	Accurate Potential Energy Surface for the 1²Aâ€² State of NH₂: Scaling of External Correlation Versus Extrapolation to the Complete Basis Set Limit. Journal of Physical Chemistry A, 2010, 114, 9644-9654.	2.5	29
114	Trajectory Surface Hopping Study of the Li + Li2(X1Î£g+) Dissociation Reaction. Journal of Physical Chemistry A, 1998, 102, 6057-6062.	2.5	28
115	On the high pressure rate constants for the H/Mu + O2 addition reactions. Physical Chemistry Chemical Physics, 2001, 3, 505-507.	2.8	28
116	MODELING AND INTERPOLATION OF GLOBAL MULTI-SHEETED POTENTIAL ENERGY SURFACES. Advanced Series in Physical Chemistry, 2004, , 205-270.	1.5	28
117	Quasiclassical Trajectory Study of Atom-Exchange and Vibrational Relaxation Processes in Collisions of Atomic and Molecular Nitrogen. Journal of Physical Chemistry A, 2010, 114, 6063-6070.	2.5	28
118	Extrapolation of Hartreeâ€“Fock and multiconfiguration self-consistent-field energies to the complete basis set limit. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	28
119	Single-Valued Double Many-Body Expansion Potential Energy Surface of Ground-State SO2. Journal of Physical Chemistry A, 2002, 106, 556-562.	2.5	27
120	Dynamics Study of the O + HO2Reaction Using Two DMBE Potential Energy Surfaces:Â The Role of Vibrational Excitationâ€. Journal of Physical Chemistry A, 2004, 108, 8721-8730.	2.5	27
121	Accurate double many-body expansion potential energy surface for triplet H3+. II. The upper adiabatic sheet (2â€Š3Aâ€²). Journal of Chemical Physics, 2004, 120, 253-259.	3.0	27
122	Accurate ab initio based DMBE potential energy surface for the ground electronic state of N2H2. Journal of Chemical Physics, 2009, 131, 044309.	3.0	27
123	N(4Sâ€‰/2D)+N2: Accurate ab initio-based DMBE potential energy surfaces and surface-hopping dynamics. Journal of Chemical Physics, 2012, 137, 22A515.	3.0	27
124	Low-temperature D+ + H2 reaction: A time-dependent coupled wave-packet study in hyperspherical coordinates. Journal of Chemical Physics, 2015, 142, 024304.	3.0	27
125	On the performance of various hierarchized bases in extrapolating the correlation energy to the complete basis set limit. Chemical Physics Letters, 2015, 641, 90-96.	2.6	27
126	Quasiclassical Trajectory Study of the Environmental Reaction O + HO2 â†’ OH + O2. Journal of Physical Chemistry A, 1998, 102, 6935-6941.	2.5	26

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127	Anatomy of the S(1D) + H2 reaction: the dynamics on two new potential energy surfaces from quantum dynamics calculations. Physical Chemistry Chemical Physics, 2011, 13, 13645.	2.8	26
128	Ab Initio Based Double-Sheeted DMBE Potential Energy Surface for N₃(²Aâ€³) and Exploratory Dynamics Calculations. Journal of Physical Chemistry A, 2011, 115, 12390-12398.	2.5	26
129	On the role of dynamical barriers in barrierless reactions at low energies: S(1D) + H2. Journal of Chemical Physics, 2011, 135, 134313.	3.0	26
130	Coupled 3D Time-Dependent Wave-Packet Approach in Hyperspherical Coordinates: Application to the Adiabatic Singlet-State(1¹Aâ€²) D⁺ + H₂ Reaction. Journal of Physical Chemistry A, 2014, 118, 4837-4850.	2.5	26
131	Coupled 3D Time-Dependent Wave-Packet Approach in Hyperspherical Coordinates: The D⁺+H₂ Reaction on the Triple-Sheeted DMBE Potential Energy Surface. Journal of Physical Chemistry A, 2015, 119, 12392-12403.	2.5	26
132	Role of (H₂O)_n (n = 2â€“3) Clusters on the HO₂ + O₃ Reaction: A Theoretical Study. Journal of Physical Chemistry B, 2016, 120, 1560-1568.	2.6	26
133	A novel accurate representation of a double-valued potential energy surface by the DMBE method. Application to triplet H3+(). Chemical Physics, 2005, 308, 285-295.	1.9	25
134	Potential Energy Surface for Ground-State H2S via Scaling of the External Correlation, Comparison with Extrapolation to Complete Basis Set Limit, and Use in Reaction Dynamics. Journal of Physical Chemistry A, 2009, 113, 9213-9219.	2.5	25
135	Quasiclassical Trajectory Study of the C(¹D) + H₂ Reaction and Isotopomeric Variants: Kinetic Isotope Effect and CD/CH Branching Ratio. Journal of Physical Chemistry A, 2011, 115, 7882-7890.	2.5	25
136	CBS extrapolation in electronic structure pushed to the end: a revival of minimal and sub-minimal basis sets. Physical Chemistry Chemical Physics, 2018, 20, 22084-22098.	2.8	25
137	Multivalued Potential Energy Surfaces for Dynamics Studies. Lecture Notes in Quantum Chemistry II, 2000, , 33-56.	0.3	25
138	J = 0 reactivity and cross-section in the H + O2 reaction: is there a pronounced maximum as a function of energy?. Chemical Physics Letters, 1995, 235, 111-118.	2.6	24
139	Accurate double many-body expansion potential energy surface for triplet H[sub 3][sup +]. I. The lowest adiabatic sheet (a[sup 3]Î£[sub u][sup +]). Journal of Chemical Physics, 2003, 118, 2637.	3.0	24
140	Recalibrated Double Many-Body Expansion Potential Energy Surface and Dynamics Calculations for HN2. Journal of Physical Chemistry A, 2007, 111, 1172-1178.	2.5	24
141	xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si88.gif" display="inline" overflow="scroll"><mml:mrow><mml:msup><mml:mrow /><mml:mrow><mml:mn>1</mml:mn></mml:mrow></mml:msup><mml:msubsup><mml:mrow><mml:mi mathvariant="normal">Î£</mml:mi></mml:mrow><mml:mrow><mml:mi>g</mml:mi></mml:mrow><mml:mrow><mml:mo>+</mml:mo></mml:mrow></mml:msubsup></mml:mrow></mml:math>	2.6	24
142	Accurate MRCI and CC Study of the Most Relevant Stationary Points and Other Topographical Attributes for the Ground-State C₂H₂ Potential Energy Surface. Journal of Physical Chemistry A, 2010, 114, 13277-13287.	2.5	24
143	The Jahn-Teller effect in the triply degenerate electronic state of methane radical cation. Journal of Chemical Physics, 2011, 135, 174304.	3.0	24
144	Toward a unified single-parameter extrapolation scheme for the correlation energy: Systems formed by atoms of hydrogen through neon. Chemical Physics Letters, 2015, 631-632, 70-77.	2.6	24

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145	Hybrid potential function for bound diatomic molecules. Journal of the Chemical Society, Faraday Transactions 2, 1980, 76, 129.	1.1	23
146	Extrapolation method for cross-section from quantum mechanicalJ= 0 reactivity: H + O2. Molecular Physics, 1995, 85, 1159-1164.	1.7	23
147	A VTST Study of the H + O3and O + HO2Reactions Using a Six-dimensional DMBE Potential Energy Surface for Ground State HO3. Journal of Physical Chemistry A, 2002, 106, 4077-4083.	2.5	23
148	Accurateab initio-based molecular potentials: from extrapolation methods to global modelling. Physica Scripta, 2007, 76, C28-C35.	2.5	23
149	Dynamics and kinetics of the H+SO2 reaction: A theoretical study. Chemical Physics Letters, 2007, 439, 301-307.	2.6	23
150	Double many-body expansion of the two lowest potential-energy surfaces for Li3 and dynamics of the Li + Li2(v) reaction. Initial orientation and vibrational excitation effects. Journal of the Chemical Society, Faraday Transactions, 1993, 89, 1511.	1.7	22
151	Potential Energy Surfaces for the Low-Lying 2A'' States of HO2 via a Multivalued Double Many-Body Expansion: Modeling Basic Attributes. The Journal of Physical Chemistry, 1995, 99, 15846-15857.	2.9	22
152	On the behavior of single-surface nuclear wavefunctions in the vicinity of the conical intersection for an X3 system. Chemical Physics Letters, 2000, 316, 248-256.	2.6	22
153	Dynamics of the OH(v = 1,2,4) + O3 atmospheric reaction. Physical Chemistry Chemical Physics, 2001, 3, 1439-1445.	2.8	22
154	On the Rovibrational Partition Function of Molecular Hydrogen at High Temperatures. Journal of Physical Chemistry A, 2001, 105, 9518-9521.	2.5	22
155	Geometrical phase effect in Jahnâ€“Teller systems: Twofold electronic degeneracies and beyond. Chemical Physics Letters, 2010, 487, 139-146.	2.6	22
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